

## Modeling of heat and mass transfer during thermal decomposition of a single solid fuel particle

IZABELA WARDACH-ŚWIĘCICKA\*  
DARIUSZ KARDAŚ

The Szewalski Institute of Fluid-Flow Machinery Polish Academy of Sciences,  
Fiszera 14, 80-231 Gdańsk, Poland

**Abstract** The aim of this work was to investigate the heat and mass transfer during thermal decomposition of a single solid fuel particle. The problem regards the pyrolysis process which occurs in the absence of oxygen in the first stage of fuel oxidation. Moreover, the mass transfer during heating of the solid fuels is the basic phenomenon in the pyrolysis-derived alternative fuels (gas, liquid and solid phase) and in the gasification process which is focused on the generation of syngas (gas phase) and char (solid phase). Numerical simulations concern pyrolysis process of a single solid particle which occurs as a consequence of the particle temperature increase. The research was aimed at an analysis of the influence of particle physical properties on the devolatilization process. In the mathematical modeling the fuel grain is treated as an ideal sphere which consists of porous material (solid and gaseous phase), so as to simplify the final form of the partial differential equations. Assumption that the physical properties change only in the radial direction, reduces the partial derivatives of the angular coordinates. This leads to obtaining the equations which are only the functions of the radial coordinate. The model consists of the mass, momentum and energy equations for porous spherical solid particle heated by the stream of hot gas. The mass source term was determined in the wide range of the temperature according to the experimental data. The devolatilization rate was defined by the Arrhenius formula. The results of numerical simulation show that the heating and devolatilization time strongly depend on the physical properties of fuel. Moreover, proposed model allows to determine the pyrolysis process direction, which is limited by the equilibrium state.

---

\*Corresponding Author. E-mail: izkaw@imp.gda.pl

**Keywords:** Fuel particle; Devolatilization; Pyrolysis; Heat and mass transfer

## Nomenclature

$A_0$	–	pre-exponential factor in the Arrhenius formula, 1/s
$c$	–	specific heat capacity, J/kgK
$d$	–	diameter, m
$E_a$	–	activation energy in the Arrhenius formula, J/molK
$H$	–	Heaviside function
$K$	–	permeability, m <sup>2</sup>
$k$	–	rate coefficient, 1/s
$n$	–	summation index
$Nu$	–	Nusselt number
$p$	–	gas pressure, Pa
$Pr$	–	Prandtl number
$r$	–	radius, radial coordinate, m
$Re$	–	Reynolds number
$\dot{S}$	–	volumetric mass source, kg/m <sup>3</sup> s
$T$	–	temperature, K
$t$	–	time, s
$u$	–	gas velocity, m/s
$U$	–	variable, $U = Tr$ , Km
$Y$	–	mass fractions, kg/kg
$Z$	–	pyrolysis progress, kg/kg

## Greek symbols

$\bar{\alpha}$	–	heat transfer coefficient, W/m <sup>2</sup> K
$\epsilon$	–	porosity, m <sup>3</sup> /m <sup>3</sup>
$\kappa$	–	thermal diffusivity, m <sup>2</sup> /s
$\lambda$	–	thermal conductivity, W/mK
$\mu$	–	dynamic viscosity, Pas
$\omega$	–	emissivity
$\pi$	–	$\pi$ number
$\Psi$	–	internal volumetric heat sources, kJ/m <sup>3</sup> s
$\rho$	–	density, kg/m <sup>3</sup>
$\sigma$	–	Stefan-Boltzmann constant, W/m <sup>2</sup> K <sup>4</sup>

## Subscripts

0	–	initial state
C	–	temperature in Celsius, coal element
H	–	hydrogen element
K	–	temperature in Kelvin
$b$	–	surface
$e$	–	equilibrium state
$eff$	–	effective values

<i>fluid</i>	–	surrounding heating medium
<i>g</i>	–	gas
<i>k</i>	–	convective
<i>p</i>	–	particle, constant pressure
<i>r</i>	–	radiative
<i>s</i>	–	solid

## 1 Introduction

Thermal decomposition of solid fuel particles plays an important role in energy generation. Solid fuels like biomass or coal may have different physical and chemical properties, depending on the growth/mining place. Therefore, the efficiency of production of gases and their composition may vary and thus operating of the reactor becomes difficult. In the case of using coal/biomass blends the situation becomes even more complex. The biomass has even three times higher volatile content and two times higher moisture content than coal. Therefore, the analysis of devolatilization of various fuels has a practical meaning. Moreover, thermal processing of solid fuel particles with mass loss phenomenon is interesting from research reasons. Due to the heat transfer from hot surrounding gases to a solid fuel, the mass transfer from particle to its neighborhood takes place. At the beginning of the heating process, water vaporizes from the particle surface. In the next phase, in a consequence of the internal energy increase, the internal particle structure changes and the volatiles are released as gases.

In the case of very small particle (e.g., pulverized coal combustion, where the particle size is reduced to an average diameter of 70  $\mu\text{m}$ ), numerical modeling is practically the only way of broadening knowledge about combustion of solid particles [1]. It gives detailed information about temperature and velocity fields inside and in the vicinity of particle. Generally, in the thermal decomposition the fuel particle is heated by hot flue gases. The rate of temperature increase and the temperature distribution inside of the particle are the functions of convective and radiative heat fluxes through the surface, particle size and the heat conductivity. Determination of the particle temperature strongly depends on the proper definition of the physical parameters and their changes during devolatilization. Additionally, the heating of the particle may cause abrupt changes of its volume [2, 3]. This phenomenon was analyzed in the case of devolatilization of pulverized coal in a hot stream of flue gases [4].

The main goal of the work was to investigate the process of thermal decomposition of a single solid fuel particle. For this purpose the simplified

one-dimensional model was developed. The influence of physical and chemical fuel properties and process parameters on the devolatilization time was emphasized.

## 2 Mathematical model of devolatilization process

In this work the thermal decomposition process of the solid fuel is studied. Numerical simulations concern pyrolysis process of the single solid particle which occurs in the absence of oxygen during particle heating. Due to the increase of internal energy of solid particle, the basic material structure changes. In result, the bonds of the long chains of hydrocarbons are breaking and the shorter chains are released as gases.

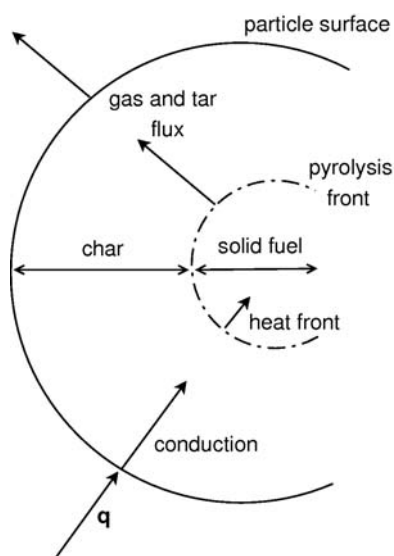


Figure 1. Scheme of the transport processes during pyrolysis.

The transport processes occur in the single stationary solid fuel particle are schematically presented in Fig 1. An increase in the local temperature from the outer surface to the core due to the heating initiates the thermal decomposition reaction in the same direction and formation of a porous char. Released volatiles diffuse through the pores in the opposite direction, to the outer parts of the particle, becoming an additional source for the gases in the vicinity of the solid fuel. Other process accompanying pyrolysis include the pressure increase inside of the particle caused by the formation

of gases, which must be high enough to overcome the flow resistance of the gas, which is associated with the porosity of the substance. In result, the diffusion of gas molecules and the shrinkage and swelling of grains take place [5].

In the studied case the single solid fuel particle is treated as an ideal sphere which consists of porous solid phase and gaseous phase. The assumption of the particle shape and, additionally, the physical quantities being varied only in the radial direction simplifies the final form of the partial differential equations. This leads to obtaining the equations which are the functions of radial coordinate only. The model consists of the mass, momentum and energy equations for porous spherical solid particle heated by the hot gas stream:

- mass balance equation for the solid phase:

$$\frac{\partial \epsilon_s \rho_s}{\partial t} = \dot{S}_s, \quad (1)$$

where  $\epsilon_s$  [m<sup>3</sup>/m<sup>3</sup>] is the volume fraction of solid phase,  $\rho_s$  [kg/m<sup>3</sup>] is the density of solid phase, and  $\dot{S}_s$  [kg/m<sup>3</sup>s] is the volumetric mass source for solid phase;

- momentum equation for pyrolytic gases:

$$\frac{\partial \epsilon_g \rho_g u}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 (\epsilon_g \rho_g u \otimes u) \right] = - \frac{\partial p}{\partial r} - \frac{\mu \epsilon_g}{K} u, \quad (2)$$

where symbol  $u$  [m/s] denotes gas velocity,  $p$  [Pa] is the gas pressure,  $\mu$  [Pas] is the dynamic viscosity, and  $K$  [m<sup>2</sup>] is the permeability;

- energy balance with the assumed local thermal equilibrium state between the phases:

$$\begin{aligned} & \frac{\partial \rho_{eff} c_{eff} T}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 (\epsilon_g \rho_g c_g T u) \right] = \\ & - p \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u) - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \left( -\lambda_{eff} \frac{\partial T}{\partial r} \right) \right] + \Psi, \end{aligned} \quad (3)$$

where  $T$  [K] is the temperature of gas and solid phase ( $T_g = T_s = T$ ),  $\lambda$  [W/mK] is the thermal conductivity,  $c$  [kJ/kgK] is the specific heat capacity,  $\Psi$  [kJ/m<sup>3</sup>s] represents the internal volumetric heat sources, and subscript *eff* denotes the effective values.

Additionally, for determination of the gas pressure the Clapeyron equation for the ideal gas is considered.

As for the initial condition, it is assumed that the following parameters are known: the apparent density of the solid phase, density of gas filling the pores, porosity of the particle, temperature of the particle, pressure of the gas inside of the pores, velocity of gases inside of the pores. Moreover, the temperature of surrounding hot gases,  $T_{fluid}$ , is known. Subscript fluid denotes the heating medium. The temperature at the particle surface (boundary condition) is calculated from the heat balance between hot surrounding gases and cold particle

$$\bar{\alpha} [T_{fluid}(t, r) - T(t, 0)] = -\lambda_{eff} \left. \frac{\partial T(t, 0)}{\partial r} \right|_{wall}, \quad (4)$$

where  $\bar{\alpha}$  [W/m<sup>2</sup>K] is an average heat transfer coefficient. The considered case concerns the forced convection (the grain is heated from the hot gas stream, which flows over the particle with the known velocity  $u_{fluid}$ ). The convective heat transfer coefficient,  $\bar{\alpha}_k$ , can be calculated from the formula [6]

$$Nu = 2 + 0.6Re^{1/2}Pr^{1/3} \quad \text{for } 1 < Re < 7 \times 10^4 \quad \text{and } 0.6 < Pr < 400, \quad (5)$$

where Nu is the Nusselt number ( $Nu = \bar{\alpha}_k d_p / \lambda_{eff}$ ), Pr is the Prandtl number ( $Pr = c_{p,fluid} \mu_{fluid} / \lambda_{fluid}$ ), and Re is the Reynolds number ( $Re = \rho_{fluid} u_{fluid} d_p / \mu_{fluid}$ ). Due to the high temperatures, the radiative heat transfer coefficient should also be taken into account

$$\bar{\alpha}_r = \sigma \omega \frac{T_{fluid}^4 - T_b^4}{T_{fluid} - T_b}, \quad (6)$$

where  $\sigma$  is the Stefan-Boltzmann constant,  $5.670 \times 10^{-8}$  W/m<sup>2</sup>K<sup>4</sup>,  $\omega$  is the emissivity, and  $T_b$  refers to the surface temperature. The average heat transfer coefficient,  $\bar{\alpha}$ , appeared in Eq. (4), can be calculated as the sum of convective,  $\bar{\alpha}_k$ , and radiative,  $\bar{\alpha}_r$ , heat transfer coefficients. Additionally, the symmetry in the center of the system is assumed (both for temperature and velocity field). The first results of the proposed mathematical model were presented in [7].

The gas mass source term caused by devolatilization is described on the basis of the following equation [8]:

$$\frac{dZ}{dt} = -k(Z - Z_e)H(Z - Z_e), \quad (7)$$

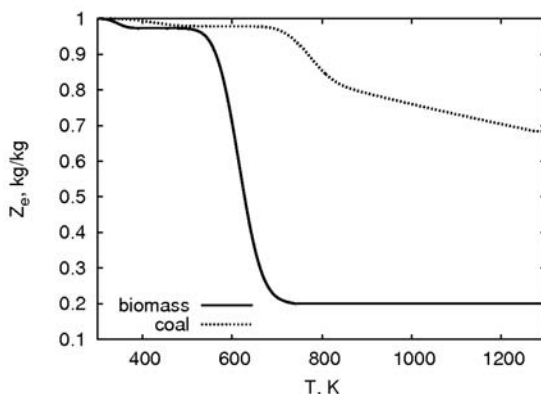


Figure 2. Equilibrium pyrolysis progress for different fuels measured during heating, thermogravimetric data [9, 11].

where  $k = k(T)$  [1/s] is the rate coefficient defined by the Arrhenius equation,  $Z$  [kg/kg] is the pyrolysis progress expressed as an instantaneous to initial mass ratio,  $Z_e = Z_e(T)$  [kg/kg] is an equilibrium function of pyrolysis progress, (Fig. 2), and  $H$  denotes the Heaviside function. The equilibrium function  $Z_e$  refers to the slow pyrolysis process, i.e., for the heating rate tending to zero. The Heaviside function allows to determine the pyrolysis process direction, which means that for the negative values, the devolatilization does not occur. Moreover, the curve described by Eq. (7) determines the available states that can be reached in real processes. Those states are defined by the area over  $Z_e$  function, the area below this function represents the unavailable states of pyrolysis. The mathematical formula for  $Z_e$  function was determined based on experimental data (Institute for Chemical Processing of Coal in Zabrze, [9]), for different types of coal and biomass (different volatile content, different particle sizes) [10, 11]. The chosen samples are presented in Fig. 2. It might be seen that the curves have a similar shape, i.e., the equilibrium particle pyrolysis progress decreases with temperature increase, so according to the definition of the pyrolysis progress presented above, also the particle mass decreases. For the case of biomass (pine chips) the most intense devolatilization process occurs at a temperature around 600 K. The values of the pyrolysis progress for biomass decrease with the increasing temperature to value of about 0.2 at the temperature over 700 K. This value is determined by the content of volatile matter, appropriate value for this type of fuel is 80% (as received). For coal (coal from Budryk mine) the most intense mass loss process occurs at around 750 K.

The curves of pyrolysis progress for coal approach the limit of about 0.68. As it was mentioned before, this value is determined basing on the content of volatile matter in this type of fuel (Budryk) which is equal to 32% (as received).

Comparing the behavior of biomass and coal fuel type during the heating process, it can be concluded that the biomass devolatilize faster than coal. Furthermore, the change of mass is larger for biomass than for coal, which is due to the higher content of volatile matter in the biomass fuel.

### 3 Numerical results of heat transfer simulations

In the first stage of the study only the heating of the pure solid phase, neglecting the devolatilization process, was considered. The main goal was to compare the numerical results derived using the commercial code ANSYS Fluent [12] with the numerical results from the in-house code. For this purpose it was assumed that the coal particle is a nonporous and spherical material with following constant physical properties: density  $\rho = 1540 \text{ kg/m}^3$ , specific heat  $c_p = 1.2 \text{ kJ/kgK}$ , and thermal conductivity  $\lambda = 0.25 \text{ W/mK}$ . The initial temperature of the particle was set to 298 K, and the surface temperature to 1273 K. In case of ANSYS Fluent, transient 3D calculations were performed. Maps presented in Fig. 3 show the temperature distribution in a homogeneous and sphere coal particle, in two different times calculated within the commercial code. It is seen that after 4.0 s the core of the particle achieves temperature of 1090 K.

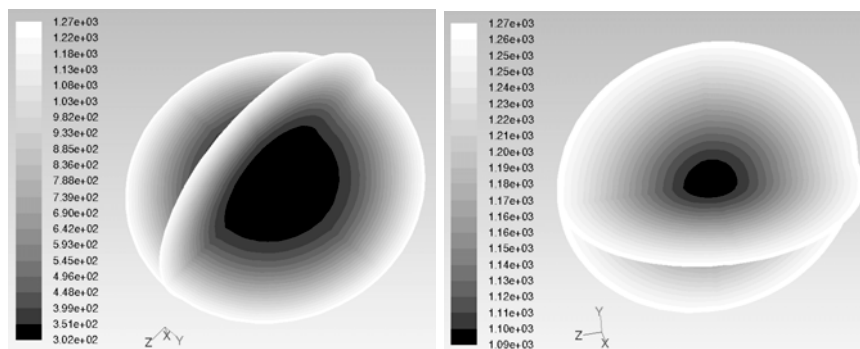


Figure 3. Temperature distribution in a coal particle with diameter 3 mm for different times: 0.5 s (left map), and 4.0 s (right map);  $T_b = 1273 \text{ K}$ .



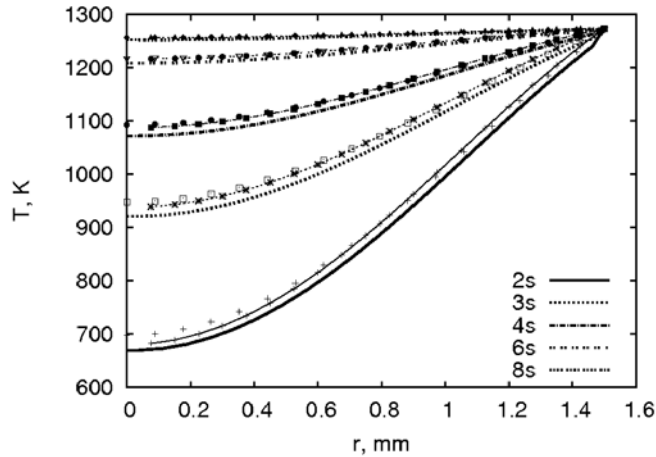


Figure 4. Temperature profiles in a coal particle with diameter 3 mm for different times and different codes: dotted lines – ANSYS Fluent 3D, solid lines – in-house code 1D, dashed-dotted lines – analytical solution [13];  $T_b = 1273$  K.

The comparison of different numerical results is shown in Fig. 4. The simulations concern presented case, i.e., the heating of the homogeneous coal particle with diameter of 3 mm. The dotted lines represent the temperature inside of the grain calculated from ANSYS Fluent, while solid lines numerical results from in-house 1D model presented above. The dashed-dotted lines illustrates the analytical solution of heating 1D radial heat flow in the sphere.

In the case of the ‘pure’ heat transfer and homogeneous material, the energy balance equation (3) reduces to

$$\frac{\partial T}{\partial t} = \kappa \left( \frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right), \quad (8)$$

where  $\kappa = \lambda/(\rho c)$ . Substituting new variable into (8),  $T = U/r$ , we can obtain the simplest form of this equation

$$\frac{\partial U}{\partial t} = \kappa \frac{\partial^2 U}{\partial r^2}, \quad (9)$$

allowing to obtain an analytical solution of radial heat flow in a sphere with a radius  $r_0$ , and surface temperature  $T_b$  [13]:

$$T(r) = T_b + \frac{2r_0 T_b}{\pi r} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \sin\left(\frac{n\pi r}{r_0}\right) \exp^{-\kappa n^2 \pi^2 t / r_0^2}. \quad (10)$$

The comparison shows the similarity between the temperatures calculated using different methods. For time 2 s the temperature in the core is equal to 698 K for ANSYS Fluent solution and 670 K for the in-house model, whereas the analytical solution gives value of 682 K. For the core temperature the calculation errors, related to the analytical solution, are 2.3% for ANSYS Fluent and 1.8% for the in-house 1D model. It should be noted, that the ANSYS Fluent 3D calculations was carried out with Cartesian coordinates. Moreover, the difference tends to zero when the temperature of the particle reaches the surface temperature. In Tab. 1 the results of numerical simulation of coal particle (porosity  $\epsilon = 0$ ) heating are presented. The heating time was defined as a time after which the average temperature of the particle was equal to 1272.40 K ( $0.9995T_b$ ). In all cases the difference in computed temperatures between commercial and in-house codes is observed. In the case of the smaller particle (1–2 mm) this difference is about 10%, whereas for the particle of 3 mm diameter this difference is only about 3%. Independently from the used model, an increase of three times of magnitude for particle size results in the heating time increase for almost ten times. Particle with diameter of 1 mm achieves the set temperature in the time about 1 s, whereas for the of 3 mm diameter this time is equal to 11 s.

Table 1. Heating time for different sizes of homogeneous particles;  $T_b = 1273$  K. Constant physical parameters for the coal.

Particle diameter [m]	Porosity [ $\text{m}^3/\text{m}^3$ ]	Heating time [s]		
		ANSYS Fluent 3D	In-house code 1D	Difference [%]
0.001	0.0	1.20	1.32	10
0.002	0.0	4.80	5.29	10
0.003	0.0	11.50	11.91	3

The results of numerical simulation of single particle heating resulting from the in-house code are presented in Tab. 2. These simulations consider only the heating without gas releasing, with assumption that the basic material is porous and consists of two phases, solid and gas, with porosity  $\epsilon_g$ . The heating time was defined as a time after which the average temperature of the particle was equal to 1272.40 K ( $0.9995T_{fluid}$ ), whereas the surrounding moving fluid with the velocity  $u_{fluid}$  has a temperature of 1273.15 K. The initial temperature of the particle was set to 300 K. It can be seen that the heating time strongly depends on the physical properties of fuel.

For biomass (wood), an increase of two orders of magnitude for the particle size results in the heating time increase of almost two thousand times. For coal this ratio has a much lower value, approx. one hundred. Therefore the heating time for coal type fuel is about half order higher than for biomass (for the same particle sizes), what results from the type and porosity of the material.

Table 2. Heating time for different single fuel particles. The velocity and temperature of surrounding gas:  $u_{fluid} = 10^{-4}$  m/s,  $T_{fluid} = 1273$  K.

Particle diameter [m]	Porosity [m <sup>3</sup> /m <sup>3</sup> ]		Heating time [s]	
	Biomass	Coal	Biomass	Coal
0.001	0.5	0.2	10.36	41.20
0.01	0.5	0.2	284.19	915.20
0.1	0.5	0.2	18 773.86	49 276.75

## 4 Devolatilization process modeling

The devolatilization process of the solid fuel is investigated. The main goal was to analyze the influence of the fuel physical properties and the particle size on devolatilization time. For this purpose numerical modeling is carried out by means of the in-house 1D code. In the studied cases the particle is treated as a spherical stationary grain flowed over by hot gases. Additionally, particle is treated as an open system where in result of heat transfer from the hot gases, the mass transfer (release of volatiles) takes place. In that stage of the simulation the volume changes are not included. For the numerical simulation the 1D spherical system is taken into account. The appropriate conditions for mass changes are obtained by different temperatures of stationary ‘cold’ grain and moving surrounding ‘hot’ gases. Fuel particle has a initial temperature of 300 K, and gases have a temperature of 1273 K. In the calculations, the thermal and physical properties of the fuel are the functions of the temperature. The pyrolytic gases are treated as a homogeneous air mixture of density being described also by the function of the temperature [14]

$$\rho_g = 344.63T^{-1.001} . \quad (11)$$

Two types of fuel were investigated: coal and biomass. It should be pointed out that this work does not consider the chemical composition of

pyrolytic gases, so the chemical composition of fuel is not taken into account. In this stage of analysis, the chemical reactions between releasing gases and surrounding gases are not considered. The more important parameters are: the fuel volatile content, which determines the additional gas source in the surrounding flow, and the porosity of the grain. For considered fuels the volatile content is 25% for coal and 62.5% for biomass. The porosity was assumed to be 0.2 for coal and 0.5 for biomass. The moisture content is equal to zero for both fuels, due to the fact that only dry fuels are analyzed. In all simulations the different size of fuel particle is considered (from 1 to 3 mm diameter). In addition, in this step of simulations the constant values of density and diameter of the particle during pyrolysis were assumed. The main initial parameters for fuels are presented in Tab. 3. The different constants for Arrhenius equation for coal (slow heating rate [15]) and biomass (very slow heating rate [16]) were used.

Table 3. Initial parameters for calculation:  $u_{fluid} = 10^{-4}$  m/s,  $T_{fluid} = 1273$  K,  $T_0 = 300$  K.

Fuel	Porosity [m <sup>3</sup> /m <sup>3</sup> ]	Apparent density [kg/m <sup>3</sup> ]	Preexponential factor [1/s]	Activation energy [kJ/kmolK]
Biomass	0.5	662.167	2 980.00	73 100.00
Coal	0.2	1 540.901	1.35	69 000.00

All other thermophysical parameters are the function of temperature. Specific heat for biomass was determined as [17]

$$c_{p,biomass}(T_K) = 0.1031 + 0.003867T_K \quad \text{kJ/kgK}, \quad (12)$$

where  $T_K$  is temperature in Kelvin. Specific heat for coal was calculated from [18]

$$c_{p,coal}(T_C) = \begin{cases} 1.15 \text{ kJ/kg} & \text{for } T_C < 300 \text{ }^\circ\text{C}, \\ 1.15 + 2.03 \times 10^{-3}(T_C - 300 \text{ }^\circ\text{C}) & \\ -1.55 \times 10^{-6}(T_C - 300 \text{ }^\circ\text{C})^2 & \\ 1.15 \text{ kJ/kg} & \text{for } T_C \geq 300 \text{ }^\circ\text{C}, \end{cases} \quad (13)$$

where  $T_C$  is temperature in Celsius. Thermal conductivity for biomass was assumed to be a constant value,  $\lambda_{s,biomass} = 0.07687$  W/mK. In the case

for coal, thermal conductivity is the temperature-dependent function [19]

$$\lambda_{s,coal} = \left[ \frac{Y_C}{1.47} + \frac{Y_H}{0.0118} \left( \sqrt{\frac{273 \text{ K}}{T_K}} \right) \right]^{-1}, \quad (14)$$

where  $Y_C$  and  $Y_H$  are the coal and hydrogen content (mass fractions) in fuel, respectively. The constant values for chemical elements were assumed:  $Y_C = 0.65$  and  $Y_H = 0.05$ .

The results of numerical simulation are presented below. Left plot of Fig. 5 presents the temperature within the coal particle of diameter 1 mm in the different times. As it is seen the surface temperature increases with time as a result of heat transfer from the hot surrounding flue gases. After over

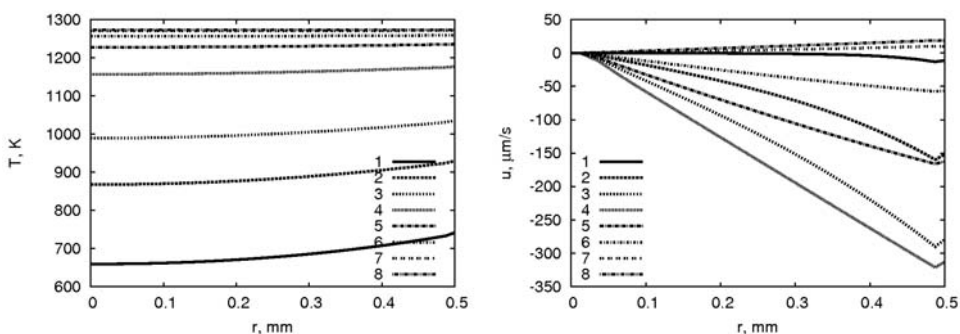


Figure 5. Temperature within the coal particle of diameter 1 mm during heating (left) and the velocity of releasing gases (right) in different times: 1–1.25 s, 2–3.75 s, 3–6.25 s, 4–12.50 s, 5–18.75 s, 6–25.00 s, 7–37.50 s, 8–62.50 s.

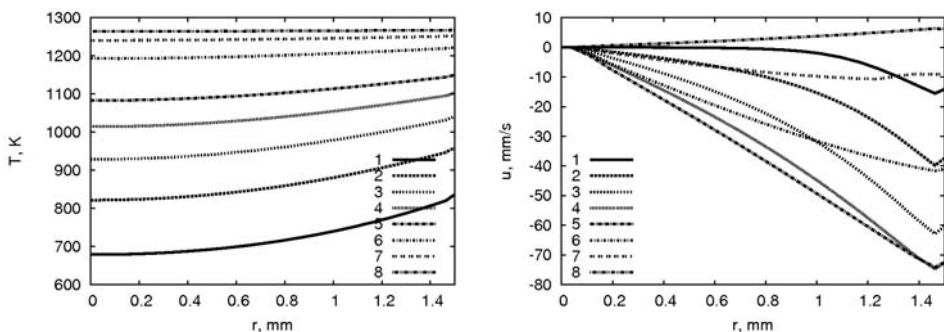


Figure 6. Temperature within the coal particle of diameter 3 mm during heating (left) and the velocity of releasing gases (right) in different times: 1–7.50 s, 2–15.00 s, 3–22.50 s, 4–30.00 s, 5–37.50 s, 6–56.25 s, 7–75.00 s, 8–112.50 s.

60 s, the surface temperature and the temperature in the core of the particle achieves the temperature of hot flue gases 1273 K. Note that the value of the velocity vector of released gases (Fig. 5 – right plot) is highly variable what affects the rate of heat propagation, and therefore the temperature distribution in grain. Moreover, at the beginning stage of the process gases are transported to the interior of the particle, which is shown by the negative sign of the velocity magnitude. After about 40 s the gases are transported to the exterior. The temperature within the coal particle of diameter 3 mm in different times is presented in the left plot of Fig. 6. In that case the temperature of the particle reaches the outside temperature after over 110 s. After that time the velocity vector of released gases (Fig. 6 – right plot) changes its sign from minus to plus, what means that gases are transported from the core to the outside. It is worth to notice that in the case of coal particle of 3 mm diameter the velocity magnitude has a two order higher value than in the case of particle of 1 mm diameter.

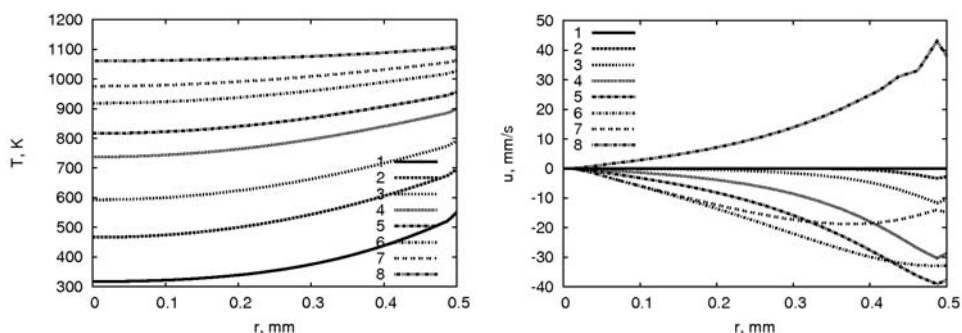


Figure 7. Temperature within the biomass particle of diameter 1 mm during heating (left) and the releasing gases velocity (right) in different times: 1–0.26 s, 2–0.38 s, 3–0.63 s, 4–1.00 s, 5–1.25 s, 6–1.63 s, 7–1.88 s, 8–2.50 s.

Left plot of Fig. 7 presents the temperature within the biomass particle of 1 mm diameter in different times. As it is seen after over 2.5 s, the average temperature of the particle increases to approx. 1080 K, so the heating time is much smaller than for coal (compare with Fig. 5). The value of the velocity vector of released gases (Fig. 7 – right plot) is highly variable; the changing of the sign of the velocity vector takes place at the end of the process, at time over 2.5 s gases are transported to the outside of the biomass grain, whereas for time less than 2.5 s gases are transported to the core of the fuel (negative sign of the velocity magnitude). The temperature within the biomass particle of diameter 3 mm, in different times are presented

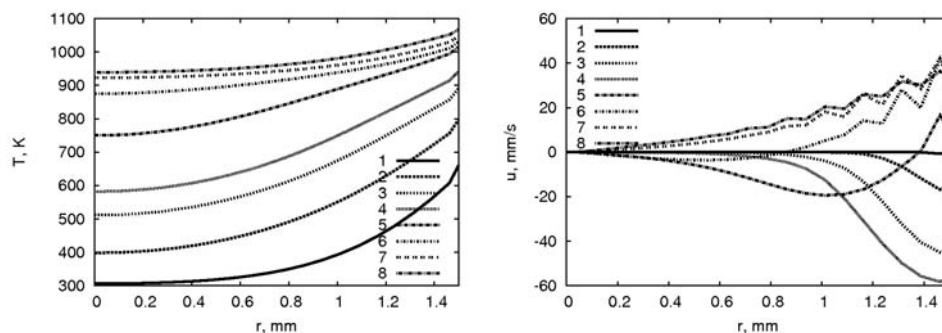


Figure 8. Temperature within the biomass particle of diameter 3 mm during heating (left) and the releasing gases velocity (right) in different times: 1–0.75 s, 2–1.88 s, 3–3.00 s, 4–3.75 s, 5–5.63 s, 6–7.50 s, 7–9.38 s, 8–11.25 s.

in Fig. 8 (left plot). In that case the average temperature of the particle after over 11 s equals approx. to 1000 K. The velocity vector of released gases (Fig. 8 – right plot) changes its sign from minus to plus after approx. 6 s, what means that gases are transported from the core to the outside of the grain. On the velocity profiles graph some numerical instabilities in the form of pitch changes of the values are observed. It comes from used explicit scheme in the discretization method.

In Fig. 9 the velocity magnitude in the distance of  $d_p/4$  from the core of the particle for different fuels and different particle sizes are presented. As it is seen, the extremum value of pyrolytic gas mixture velocity characterizing the flow direction change is achieved in time of approx. 25–50 s for coal (depending on the particle size, left plot). In the case of biomass this time is within the range from 2 to 6 s, which is a much lower value. Moreover, the total transport time of gases (500 s) is much longer for coal than for biomass (13 s).

The results presented in Tab. 4 concern the time of thermal conversion process for different type of fuel (coal and biomass) and different particle sizes. In each case the time of devolatilization is different — larger particle needs more time to lose its volatiles. Moreover, in general the coal particle devolatilizes longer than biomass one. This results from different values of physical parameter (Tab. 3) and different mass loss rate (Fig. 2). The apparent density and thermal conductivity for dry coal have over two times higher values than for dry biomass. The specific heats for this solids in the temperature of 300 K have almost the same values. The most intensive process of volatiles release for biomass takes place at lower temperatures

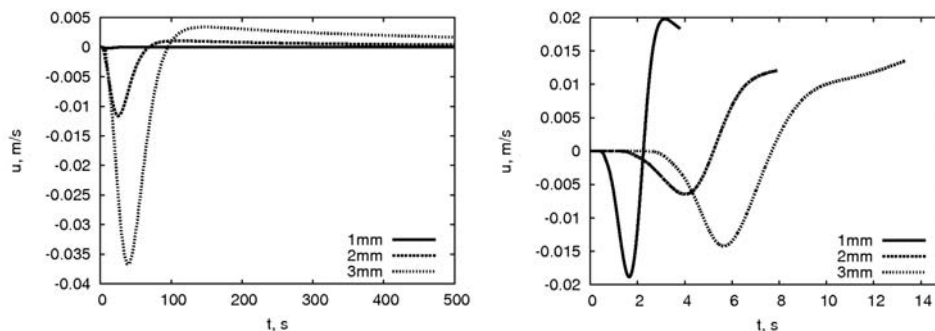


Figure 9. The velocity magnitude in the distance of  $d_p/4$  from the particle core for different fuels and different particle sizes: left – coal, right – biomass.

than for coals. Moreover, the porosity of the biomass particle is larger than for coal, what contributes to lower gas flow resistance and more intense mass loss process. The numerical results from the in-house code and the numerical results of simulation of thermal decomposition obtained by other authors [20] (Tabs. 4 and 5) are to large extent in good qualitative agreement. For the reference data with the particle size of 7.5 mm the authors obtained the ratio of decomposition time for coal to biomass at the level of 43.80 (the 90% of conversion), whereas for own cases studied herein the ratios are equal to 213, 101, and 47 for diameter 1, 2, and 3 mm, respectively. The coal to biomass time conversion ratio in performed simulations decrease with increasing particle size. It follows that in the case of diameter of 7.5 mm and for the same initial and boundary conditions, the similar range of devolatilization times would be obtained. In general, the fuel physical parameters and its particle size strongly affect the heating and devolatilization times.

Table 4. Conversion time for different single fuel particles. The velocity and temperature of surrounding gas:  $u_{fluid} = 10^{-4}$  m/s,  $T_{fluid} = 1273$  K. Initial temperature of fuel  $T_0 = 300$  K.

Particle diameter [m]	Porosity [m <sup>3</sup> /m <sup>3</sup> ]		Conversion time [s]			
	Biomass	Coal	100% conversion		90% conversion	
			Biomass	Coal	Biomass	Coal
0.001	0.5	0.2	3.80	804.72	3.00	641.38
0.002	0.5	0.2	7.90	829.48	6.13	662.50
0.003	0.5	0.2	13.35	864.41	9.44	690.00



Table 5. Conversion time for single fuel particle. The initial temperature of fuel  $T_0 = 488$  K. Temperature of surrounding gas:  $T_{fluid} = 1273$  K [20].

Parameter	Fuel	
	Biomass	Coal
$\rho$ [kg/m <sup>3</sup> ]	700	900
$\lambda$ [W/mK]	0.14	0.19
$c_p$ [J/kgK]	1500	1150
$d_p$ [m]	Time of 90% conversion [s]	
0.0075	21.00	920.00

## 5 Summary

In this work the heat and mass transfer during thermal decomposition of the single solid fuel particle were investigated. The analysis was based on the mathematical modeling of the pyrolysis process of the single solid fuel particle. The mass source term was determined in the wide range of temperature according to the experimental data and the Arrhenius equation for devolatilization rate. The two types of dried fuels were considered, namely coal and biomass with different volatiles content. Additionally, different particle sizes were investigated.

The simulation results show the importance of appropriate physical data implementation, especially the pyrolysis kinetic rate and the physical properties of the material, in thermal decomposition process calculations. It follows from the performed analysis that the intensity and time of the devolatilization process depend on the physical properties of the fuel and particle size. The devolatilization time for biomass, obtained from numerical simulations, is much lower than for coal. Moreover, the velocity vector is changing its sign during heating; at the first stage of the process the gases are transported to the core of grain, and at the second stage they flow out of the particle. This affects the time of volatiles release and the process of heat propagation.

**Acknowledgments** This work was partially supported by the system project “InnoDoktorant – Scholarships for PhD students, 4th edition” which is cofinanced by the European Union in the frame of the European Social

Fund and by the National Projects: POIG.01.01.02-24-017/08 “Smart Coke Plant Meeting the Requirements of Best Available Techniques” cofinanced by the European Regional Development Fund and POIG.01.01.02-00-016/08 “Model agroenergy complexes as an example of distributed cogeneration based on a local renewable energy sources”.

Received 28 March 2013

## References

- [1] KUROSE R., WATANABE H., MAKINO H.: *Numerical simulations of pulverized coal combustion*. KONA Powder Part. J. **27**(2009), 144–156.
- [2] FU Z., GUO Z., YUAN Z., WANG Z.: *Swelling and shrinkage behavior of raw and processed coals during pyrolysis*. Fuel **86**(2007), 418–425.
- [3] TOMCZEK J.: *Coal combustion*. The academic scripts **1667**. Silesian University of Technology, Gliwice 1992 (in Polish).
- [4] WARDACH-ŚWIĘCICKA I., KARDAŚ D., POZORSKI J.: *Modelling of interactions between variable mass and density solid particles and swirling gas stream*. J. Phys. Conf. Ser., EIOP Publishing Ltd. ETC13 **318**(2011), 13/11.
- [5] TUCK A.R.C., HALLET W.L.H.: *Modelling of particle pyrolysis in a packed bed combustor*. Tech. Rep., University of Ottawa, Ontario 2004.
- [6] ICIEK J., KAMIŃSKI W., KUDRA T., MARKOWSKI A.: *The heat transfer calculations*. The academic scripts, Technical University of Łódź, Łódź 1993 (in Polish).
- [7] WARDACH-ŚWIĘCICKA I., KARDAŚ D.: *Modeling of solid fuel particles combustion*. Proc. Int. Symp. on Turbulence, 7th, Heat and Mass Transfer, CD, ISBN 978-1-56700-302-4, Palermo 2012.
- [8] KARDAŚ D.: *Model of the coal and biomass pyrolysis rate in the non-equilibrium thermodynamic state*. Tech. Rep. IF-FM PAsci. 227/2010, Gdańsk 2010 (in Polish).
- [9] ŚCIAŻKO M.: *Modeling of pressure generation from the thermally plastified packed bed coal grains*. Tech. Rep. IChPC, Zabrze 2005 (in Polish).
- [10] POLESEK-KARCZEWSKA S.: *Comparative analysis of the kinetics of gasification of different types of biomass and fossil fuels*. Tech. Rep. IF-FM PAsci. 141/2008, Gdańsk 2008 (in Polish).
- [11] KARDAŚ D., POLESEK-KARCZEWSKA S.: *Description and solution of one-dimensional unsteady biomass pyrolysis problem in the reactor*. Tech. Rep. UWM, Olsztyn 2013 (in Polish).
- [12] *ANSYS Fluent 12.0 Tutorial Guide*. Updated for ANSYS Fluent 12.1, ANSYS, Inc., 2009.
- [13] CARSLAW H.S., JAEGER J.C.: *Conduction of heat in solids*. Oxford UP, Ely House, London 1959.
- [14] KALINOWSKI E.: *Heat transfer and heat exchangers*. Oficyna Wydawnicza Politechniki Wrocławskiej, Wrocław 1995 (in Polish).

- [15] ŚCIAŻKO M.: *Coal classification models — thermodynamic and kinetic approach*. Wydawnictwa AGH, Kraków 2010 (in Polish).
- [16] YANG Y.B., YAMAUCHI H., NASSERZADEH V., SWITHENBANK J.: *Effects of fuel devolatilisation on the combustion of wood chips and incineration of simulated municipal solid wastes in a packed bed*. *Fuel* **82**(2003), 2205–2221.
- [17] ROSS R.J. (Ed.): *Wood Handbook, Wood as an Engineering Material*. Forest Products Laboratory, United States Department of Agriculture Forest Service, Madison, Wisconsin 2010.
- [18] HEIDENREICH C.A., YAN H.M., ZHANG D.K.: *Mathematical modelling of devolatilization of large coal particles in a convective environment*. *Fuel* **78**(1999), 557–566.
- [19] SPEIGHT J.G.: *Handbook of Coal Analysis*. John Wiley & Sons, Inc., New Jersey 2005.
- [20] NAVARRO M.V., MARTINEZ J.D., MURILLO R., GARCIA T., LÓPEZ J.M., CALLÉN M.S., MASTRAL A.M.: *Application of particle model to pyrolysis. Comparison of different feedstock: Plastic, tyre, coal and biomass*. *Fuel Process. Tech.* **103**(2012), 1–8.