Model of heating and incineration of waste material single particle

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Abstract

Two kinds of fuel particles were taken for modelling: beech wood and coke particles without any degassing process. Two processes were analyzed: heating of wood particles without a chemical reaction and heating of coke particles with exothermic and endothermic reactions. The analysis concentrated on the influence of physical and chemical properties of fuel (density, heat conduction coefficient, heat capacity) on the temperature changes taking place on the surface and inside particles. The ranges of properties subject to the analysis were typical of solid waste. The analysis of unstable heating of fuel (or waste) single particle and physical and chemical processes of selected endo and exothermic reactions, presented in this paper, was developed by the author and implemented in an EXCEL application. The model gives unlimited possibilities to carry out calculations of various variants with different input data relevant to the material properties of waste substances, as well as to thermal processes conditions. The issue of a single particle incineration on the grate of a waste incineration device is the part of an elaborated model described in the paper [1].

Streszczenie

Model nagrzewania i spalania pojedynczego ziarna paliwa formowanego na bazie odpadów stałych

Praca obejmuje przegląd literaturowy modeli spalania pojedynczego ziarna paliwa stałego wraz z opracowaniem modelu spalania pojedynczego ziarna paliwa stałego formowanego na bazie odpadów stałych w dwóch wariantach:

- nagrzewanie pojedynczego ziarna paliwa bez reakcji chemicznej,

- nagrzewania pojedynczego ziarna z reakcją endotermiczną i egzotermiczną.

W obu przypadkach proces odgazowania został pominięty. Pierwszy wariant obliczeń obejmował przypadek nagrzewania jednorodnej kuli bez wewnętrznych źródeł ciepła, o początkowej wyrównanej temperaturze przeniesionej nagle w ośrodku o danej temperaturze przy czym znany był współczynnik wnikania ciepła α. . W obliczeniach symulowano wpływ zmian właściwości fizyko-chemicznych paliwa takich jak: gęstość,

współczynnik przewodzenia ciepła i pojemność cieplna (wielkości te zostały zawarte w przedziałach odpowiadających wartościom dla różnych odpadów) na czas i temperaturę nagrzewania. Podczas rozważania nagrzewania ziarna bez reakcji chemicznej brano pod uwagę jedynie przepływ ciepła obejmujący wnikanie ciepła od ośrodka do ziarna oraz przewodzenie ciepła w głąb analizowanej cząstki. W wariancie drugim w procesie wnikania ciepła uwzględnione zostały ponadto reakcje występujące na powierzchni ziarna i wewnątrz pór. Bilans cieplny został wzbogacony poprzez wprowadzenie entalpii reakcji dla dwóch odrębnych przypadków: reakcji egzotermicznej i endotermicznej.

1. Introduction

This paper presents a review of literature dealing with the combustion of a single solid fuel particle, as well as a model of combustion of solid waste particle. Two cases were analysed:

- Heating of a single fuel particle without chemical reaction,

- Heating of a single fuel particle with endothermic and exothermic reactions.

- The degassing process was omitted in this analysis.

The first version of calculation was dedicated to the heating process of a sphere of diameter 2R with no inner heat sources and with uniform initial temperature tp placed in the surrounding volume of temperature toś. The assumption was that the convection heat transfer coefficient α was known and constant. The calculation procedure was based on the paper [2]. Following parameters of a solid waste particle were taken into account: density, heat condustion coefficient, heat capacity, and their influence on the heating time and temperature was shown. It was observed that the increase of heat capacity and density of the particle increases the heating time while the increase of heat conduction coefficient leads to the opposite effect [3]. The influence of heat conduction coefficient on the temperature history inside the particle is shown on Fig.1 (apparent density 2000kg/m3, heat capacity 1000 J/kg K, volume temperature 9000C).

2. The algorithm of process of heating and combustion of coke particle with a chemical reaction

While calculating the heating of a particle without chemical reaction (version 1), only the heat transfer process from the surrounding volume and heat conduction inside the particle were taken into consideration. In the second case, the heat effect of chemical reaction inside porous surface of the particle was added for the endothermic and exothermic reactions.

Heat balance for heating and combustion of a single coke particle is shown on Fig.2. The basis of the analysis is the Fourier equation in one dimensional form:

$$\frac{\partial^2 t}{\partial x^2} + \frac{m}{x}\frac{\partial t}{\partial x} = \frac{1}{a}\frac{\partial t}{\partial \tau}$$
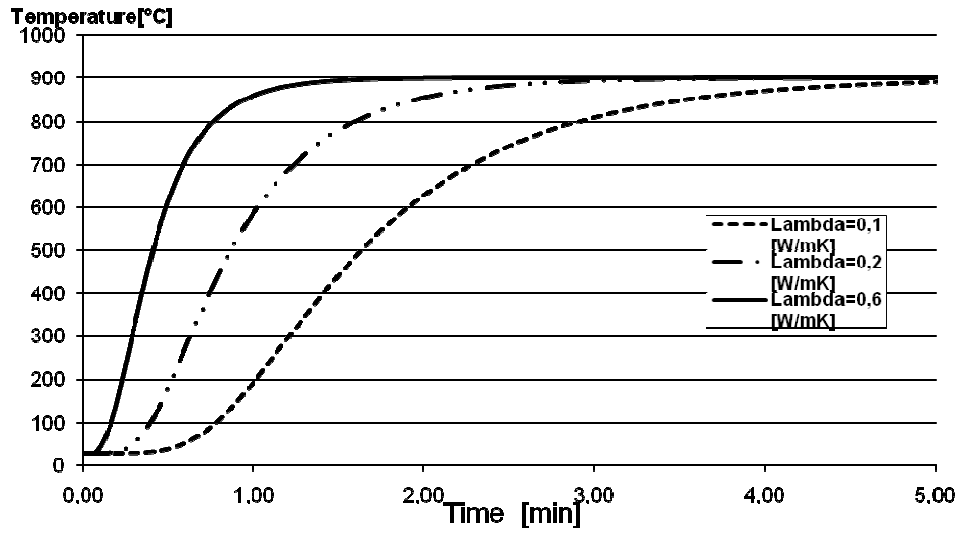
(1)

Where: m=0, 1, 2.

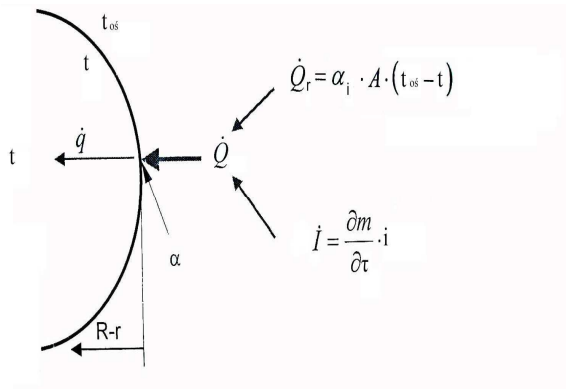Fig.1. The heating history of a particle of diameter 10mm for various heat conduction coefficients [3].

Figure 2. Heat balance of coke particle.

For the case of sphere the equation can be transformed to the form:

$$\frac{\partial t}{\partial \tau} = a\left(\frac{\partial^2 t}{\partial r^2} + \frac{2}{r}\frac{\partial t}{\partial r} \right) \qquad (2)$$

For heating process of the coke particle without chemical reaction the convective heat transfer from the surrounding gas to the surface of the particle and heat conduction to the inside volume of the particle were taken into account. The combustion process introduces additional elements to this equation – chemical reactions enthalpies on the outer surface and inside the porous surface of the particle.

Mass change of the coke particle was determined from the equation for the reaction rate. The radiation heat and chemical reaction heat create heat rate causing the increase of surface temperature and a new Biot number calculation.

Presented model shows shrinking of the reacting surface of the coke particle with constant amount of ash; therefore, this model can be described as a model of gradual conversion [4]. The heat transfer calculations were performed accordingly [2]. The concurrent mass transfer process can be represented mainly as a mass reduction resulting from carbon combustion, which was described in details in [3]. Only an outline of rough algorithm of mass transfer in a single coke particle with the exothermic reaction is presented below. Similar algorithm was created for endothermic reaction $C + H_2O \rightarrow CO + H_2$.

3. Model with the exothermic reaction $C + O_2 \rightarrow CO_2$

The chemical enthalpy changes along with the chemical reaction rate. To determine instantaneous enthalpy of reaction I, one must know the ratio $\dfrac{\partial m}{\partial t}$ and the enthalpy of unit mass i:

$$\dot{I} = \frac{\partial m}{\partial \tau} \cdot i \tag{3}$$

The standard enthalpy of reaction I_p^o is defined as a change of enthalpy of substrates transformed to products in standard parameters [5]:

$$\dot{I}_p^0 = \sum_{product} v_i' \cdot (Mi^0)_i - \sum_{substrate} v_j'' (Mi^0)_j \tag{4}$$

The elements on the right hand side of the equation are standard molar enthalpies of products and substrates multiplied by stoichiometric coefficients v of the chemical equation. As a rule, the coefficients for substrates are negative and for products are positive.

The values of standard enthalpies for many reactions were determined in various temperatures and these values should be used in precise calculations. If no precise data is accessible, the values of standard enthalpies can be determined on the basis of heat capacity and values of enthalpy in other temperatures according to relation:

$$\dot{I}_p = \dot{I}_p^0 + \Delta c_p \cdot (T_2 - T_1) \tag{5}$$

Where Δc_p is the difference of molar heat capacities of products and substrates in standard parameters with their stoichiometric coefficients, as shown in the equation:

$$\Delta c_p = \sum_j \nu_j \cdot c_{p,mj}(T) \tag{6}$$

The approximate relation was applied for calculation of $c_{p,mj}$ [6].

$$c_{p,mj} = a + bT - \frac{c}{T^2} \tag{7}$$

Coefficients a,b and c are not temperature dependent and are given in literature [6].

For the analyzed exothermic reaction, the relation (7) has the form:

$$\Delta_R c_p = c_{p,CO_2}(T) \cdot M_{CO_2} - c_{p,sC}(T) - c_{p,O_2}(T) \cdot M_{O_2} z$$

$$c_{p,sC}(T) = 16{,}86 + 4{,}77 \cdot 10^{-3} \cdot (t+273) - \frac{8{,}54 \cdot 10^5}{(t+273)^2} \tag{8}$$

The time dependent standard mass enthalpy of reaction can be calculated from the relation;

$$i = \frac{\dot{I}_p}{M_{koks}} \tag{9}$$

The mass rate in equation (3) can be calculated from the equation for the rate of reaction. Mass balance of the particle with chemical reaction and oxygen diffusion to its surface determining the combustion rate can be calculated from the equation for the rate of reaction:

$$\dot{r}_{koks,O_2} = \frac{\partial m_{koks}(t)}{\partial \tau} = -k_{koks,O_2,ef} \cdot m_{koks}(t) \cdot M_{koks} \cdot c_{O2}^m \tag{10}$$

Where: $m_{koks}(t)$- coke mass kg in the time t,

M_{koks}- molar mass of coke approximated by molar mass of carbon $M_{koks}=M_c$,

C_{O2}- oxygen concentration in the surrounding gas volume $\left[\dfrac{mol}{m^3}\right]$, taken as constant and calculated from CLAPEYRON equation, $k_{koks,O_2,ef}$ - substitute reaction rate constant,

m – dimensionless reaction order m = 0,59.

The data for kinetics are determined according to the literature [6].

Supposing that the reaction is performed for ideal gas, the amount of oxygen can be calculated from CLAPEYRON equation:

$$p \cdot V_{O2} = R \cdot T \cdot n_{O2} \tag{11}$$

And $n_{o2} = \dfrac{p \cdot V_{O2}}{R \cdot T}$ [mole].

The concentration of oxygen in the gas volume is:

$$c_{O2} = \frac{n_{O2}}{V_{air}} = \frac{p}{R \cdot T} \cdot \frac{V_{O2}}{V_{air}} \qquad (12)$$

Where: p – atmosphere pressure p=1,0125·10^5 [Pa],

T – gas medium temperature T=1173 [K],

R – universal gas constant

R= 8314,7 J/kmol K

V_{O2}- oxygen concentration in air $V_{O2} = 0,21$.

In the combustion zone controlled by kinetics of reaction the substitute coefficient of reaction rate can be defined as follows:

$$k_{koks,O_2,ef} = \eta \cdot k_{koks,O_2} \qquad (13)$$

where: η- pore affectivity as a function of Thiele module.

As the reaction proceeds, the oxygen concentration on the surface of the particle becomes equal approximately to the concentration in the gas volume; the concentration of gas products of reaction in the boundary layer decreases and in the zone of diffusion the substitute reaction constant equals to:

$$k_{koks,O_2,ef} = \beta \cdot a_p \cdot c_{O_2}^{1-m} \qquad (14)$$

where β-coefficient of mass transport, a_p-particle surface area calculated for the unit mass [m^2/kg].

The substitute reaction rate constant is determined similarly to the resistance of kinetic and diffusion in row:

$$k_{koks,O_2,ef} = \cfrac{1}{\cfrac{1}{\eta \cdot k_{koks,O_2}} + \cfrac{1}{\beta \cdot a \cdot c_{O_2}^{1-m}}} \qquad (15)$$

Where the first element represents kinetics term and the second diffusion term of reaction.

The chemical reaction rate coefficient is calculated according to Arrhenius relation. The coefficients of the equation are determined according to literature data [6] with the activation energy equal to E=139100 $\left[\dfrac{J}{mol}\right]$, pre-exponential coefficient k_0 $k_0=$

$$4,8 \cdot 10^9 \left[\frac{mol_{koks}}{kg \cdot s} \cdot \left(\frac{m^3}{mol_{O_2}} \right)^m \right]$$, and m=0,59[-]. T_{koks}- is instantaneous temperature of coke

particle surface in consecutive time step T_{koks}=t (x,τ)+273K.

The above described calculations of mass transfer coefficients, along with those mentioned in the paper [3], give the value of $k_{koks,O_2,ef}$ from eq. (15) and the rate of reaction

$\dot{r}_{koks,O_2}$ from eq. (10).

In the first time step the initial mass of the spherical particle should be calculated with the assumption that it represents about 22% of wood mass from the equation:

$$m_{koks}(t_0) = 0,22 \cdot m_{wood} = 0,22 \cdot \frac{\pi}{6} \cdot d_p^3 \cdot \rho_{wood}$$

In the next time steps the coke mass is determined from equation (10) for reaction rate for the previous time step.

Figures 3 and 4 illustrate this analysis.

Endothermic reaction $C + H_2O \rightarrow CO + H_2$

The rate of chemical endothermic reaction and subsequent coke mass loss in time was calculated according to the relation (16).

$$\dot{r}_{koks,H_2O} = \frac{\partial m_{koks}(t)}{\partial t} = -k_{koks,H_2O} \cdot A_{koks}(t) \cdot M_{koks} \cdot c_{H_2O} \tag{16}$$

4. Discussion

The final comparison of average temperature of coke particle without and with a presence of chemical reaction is shown in Fig. 3. As it was obvious, the presence of a chemical reaction on the surface increases the heating rate of the inner volume of the particle.

After about 8 seconds, the temperature in the centre of the particle (exothermic reactions) is equal to the temperature of the surrounding volume (900^0C).

With no chemical reaction, this time is about 14 seconds.

At the beginning of heating, the heat rate Q_r, coming from the surrounding volume (convection and radiation), is about 4 seconds higher for the time than the heat of endothermic reaction. As the time passes, the heat rate Q_r is reduced by the chemical reaction and, after about 20 seconds, the inner temperature of the particle reaches the surrounding temperature.
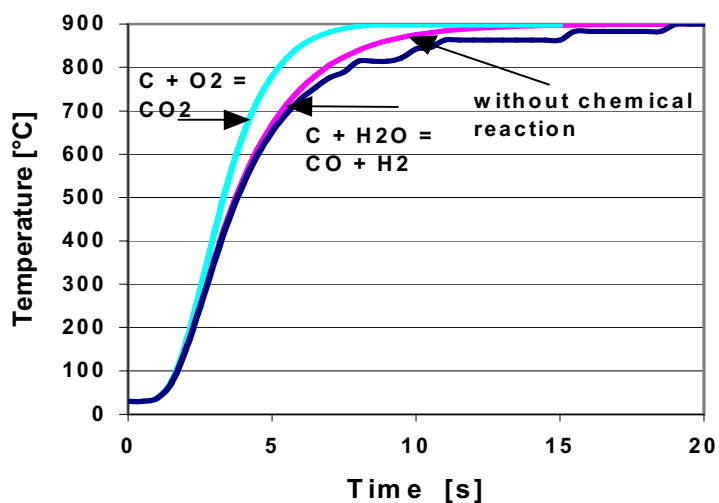
Figure 3. The time function of temperature of coke particle d=0,01 [m] for the heating process without a chemical reaction and with exothermic and endothermic reactions.
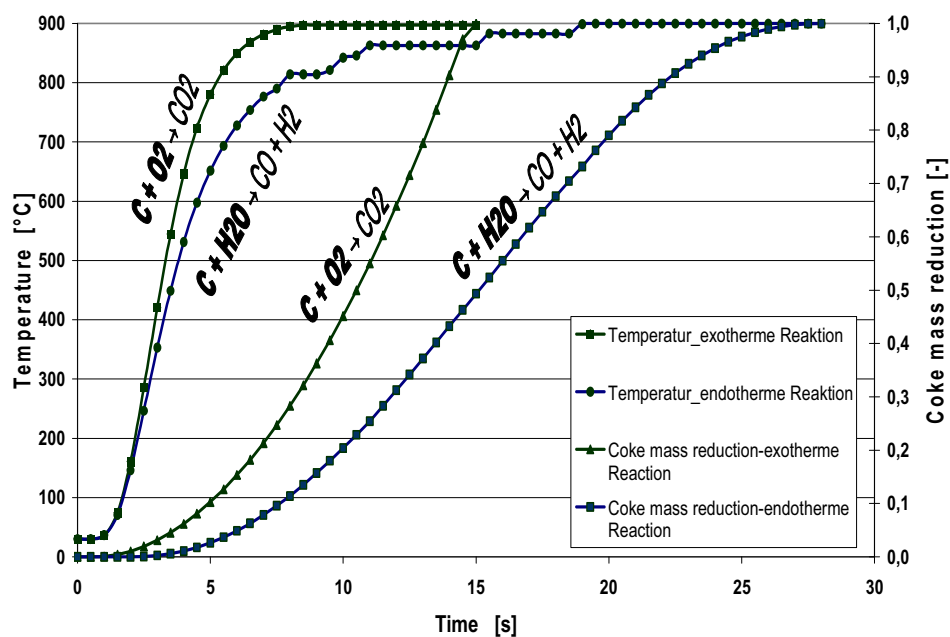

Figure 4. The time function of temperature inside the coke particle and mass reduction with exothermic and endothermic reactions [3].

5. Conclusions

The analysis presented above was carried out for two types of particle material - beech wood and coke particles without the degassing process. Two processes were analyzed: heating of the particle without chemical reaction and with exothermic and endothermic chemical reactions. As it was easy to predict, the exothermic reaction increased the heating rate of the particle in comparison with a process without the reaction. Endothermic reaction

increases the time of heating of the particle. As far as the influence of material of the particle is concerned, the heating time of the coke particle is about 14s and, for beech wood, this time is much longer (about 100s).

The influence of physical and chemical parameters of the fuel was simulated: density, heat conduction coefficient, heat capacity of the material. The values of these parameters were chosen in the range of solid waste material. The increase of heat capacity, as well as, density of material prolongs the heating time and, vice versa, the increase of heat conduction coefficient decreases the heating time of the particle.

6. Terminology

a- coefficient in heat capacity equation

b- coefficient in heat capacity equation

c- heat capacity of a substance

d- diameter[m]

i- specific enthalpy of gas [kJ/kmol]

k- chemical reaction constant []

m- mass [kg]

n- number of substances [mol]

p- pressure [Pa]

r- radius of a single particle [m], Speer of chemical reaction

t- temperature [o C]

A- area [m2]

E- activation energy

I – total enthalpy [kJ/kmol]

M- molar mass of a substance [kg/kmol]

R - universal gas cons universal J/kmol K

T- temperature [K]

V- concentration

Greek symbols

β-coefficient of mass transport []

Δ− increase[-]

η- pore efficiency [-]

ν− stoichiometric coefficient

τ− time [s]

Subscripts

O-standard state

/ // - products, substrates

m- reaction row

Superscripts

i, j- products, substrates

o- initial state

p- pressure, particle

coke-coke

o2- oxygen

ef-effective

air-air

Criteria numbers

Bi- Biot number [-]

References

[1] Jaworski T.J.,"Modelling of mass transfer process a fuel layer and the grate of waste incineration furnance". Second International Symposium on Energy from Biomass and waste.File:053. CISA Environmental Sanitary Engineering Centre, Venice, Italy, 2008.

[2] VDI-Wärmeatlas: Wärmeübergang und Strömung in Verfahrenstechnik und Chemie, version CD-ROM 1997.

[3] Jaworski T.J. "Model of combustion process of asingle particie of waste material", Feuel from Waste.Volume VI. p.91-99.Helion, Poland.Gliwice 2007.

[4] Levenspiel, O.: „Chemical Reaction Engineering".John Wiley & Sons Verlag, 3 Auflage 1999,

[5] Atkins P.W.: Chemia fizyczna, Wydawnictwo Naukowe PWN, Warsow 2001.

[6] Zelkowski J., Kohleverbrennung, Fachbuchreihe Kraftwerkstechnik. Band 8, 1. Aufl., VGB-Verlag Essen 1986.