Transactions of the VŠB – Technical University of Ostrava, Mechanical Series
No. 3, 2009, vol. LV
article No. 1733

Radim PALUSKA [*], Marian BOJKO [**], Jiří HORÁK[***]

DETERMINATION OF PULVERIZED COAL THERMOKINETIC PROPERTIES WITH USE OF MATHEMATICAL MODELLING

STANOVENÍ TERMOKINETICKÝCH VLASTNOSTÍ UHELNÉHO PRÁŠKU S POUŽITÍM MATEMATICKÉHO MODELOVÁNÍ

Abstract

Thermokinetic properties as a mean for better understanding the nature of combustion process, can be determined by experiment using the Drop Tube Test Facility (DTTF) described further in the text. DTTF provides conditions occurring in pulverized coal fired boiler by emulated oxygen concentration, temperature and velocity of reaction gas. The DTTF presented in the paper was built recently at the Energy Research Center. Experimental data acquired from DTTF are planned to be used in mathematical modelling using the code Fluent. The paper describes in detail main differences between used Fluent models of particles combustible fraction and reaction rate. Temperature field and distribution of species mass fraction is evaluated for comparing with experimental tests. Results from adjusted mathematical model should provide closer information about combustion process in real operation.

Abstrakt

Termokinetické vlastnosti, které mohou napomoci lepšímu pochopení spalovacího procesu, mohou být snadno stanoveny provedením experimentálních zkoušek na pádové trubce. Toto zařízení simuluje podmínky panující v práškovém ohništi velkých uhelných bloků nastavením základních okrajových podmínek, kterými jsou koncentrace kyslíku, teplota a rychlost reakčního plynu. Tento článek představuje pádovou trubku, která byla postavena během posledních let na Výzkumném energetickém centru. Experimentální data budou použita pro nastavení vstupních parametrů, se kterými počítá matematický model vyhořívání uhelných částic definovaný v programu Fluent. V tomto příspěvku jsou detailně popsány matematické modely spalování prchavé složky a fixního uhlíku. Tyto modely se liší v definici rychlosti chemické reakce. Teplotní pole a distribuce hmoty jsou vyhodnoceny na základě srovnání s experimentálními testy. Výsledky z nastaveného matematického modelu by měly poskytnout bližší informace o spalovacím procesu v reálném provozu.

1 EXPERIMENTAL STAND FOR DETERMINATION OF PULVERIZED COAL THERMO-KINETIC PROPERTIES

Determination of pulverized coal thermo-kinetic properties can be easily carried out with help of experimental facility called drop tube [1]. This stand (see Fig. 1) allows simulation of conditions which occur in pulverized coal-fired boiler which burn pulverized coal under exactly given boundary conditions as are temperature, concentration of oxygen and flow velocity of reaction gas in reaction chamber [2]. The result of the experiment is then so called burn-out curve, which characterises properties of given fuel during the process of burning in oxidation reactive medium.

In order to achieve the most precisely setting of boundary conditions of whole fuel burn-out process was built complete system. This system consists from reaction gas preparing, heating and

[*] Ing. Radim Paluska, Výzkumné energetické centrum, 17. listopadu 15, 708 33, Ostrava Poruba, tel. (+420) 59 732 3845, radim.paluska@vsb.cz

[**] Ing. Marian Bojko, Ph.D, VŠB - Technická univerzita Ostrava, 17. listopadu 15/2172, 708 33, Ostrava Poruba, tel. (+420) 59 732 4385, radim.paluska@vsb.cz;

[***] Ing. Jiří Horák Ph.D, Výzkumné energetické centrum, 17. listopadu 15, 708 33, Ostrava Poruba, tel. (+420) 59 732 3869, jirka.horak@vsb.cz

keeping temperature on required level within reaction chamber. At the end of sample trajectory is situated instant cooling and sampling section (see Fig. 2). System is divided in 5 sections. Major parts of components are controlled in automatic regulation by PLC unit via visualization on PC station.

I. Reaction gas preparation on desired oxygen concentration and flow rate
II. Heating of reaction gas mixture on desired temperature
III. Reaction chamber
IV. Fuel probe batching into the reaction chamber
V. Sampling with simultaneous cooling of probe on temperature under 50 °C

Reaction gas can be set on oxygen concentration ranging from 0 to 21 $\%_{vol.}$ This gas results from air which is supplied by a blower through a dust particle filter being mixed with CO_2 supplied from a bundle of pressure cylinders. A proportional amount of CO_2 and air is controlled against the required concentration of O_2 and actual value of O_2, which is determined in the analyzer (in a paramagnetic way). Both gases jointly enter through reduction valves in a blender where they are mixed. Prepared gas flows through reaction gas heater with built-in heating resistance spirals, at the beginning in first stage where is gas preheated on temperature up to 600 °C. Then gas passes through main heater in which can be warmed up to 1200 °C. After heating on required temperature enters reaction gas the drop tube reaction chamber within the velocity range of 1 - 4 m.s-1 in accordance to operating staff orders.

Vertically hinged, electrically heated 4800 mm long metal reaction chamber with inner diameter of 66 mm is manufactured from Kanthal APM (Fe75Cr20Al5). This material is able in the long term resist high temperatures in oxidation environment. Eight batching holes (with distance 500 mm from each others) are situated on sides of the drop tube in which water cooled batching unit charges a fuel sample. Distance between these batching holes and the sampling point coupled with velocity of reaction gas gives residence time of pulverized coal particle in reaction chamber.

The whole batching facility feeder and a batching probe is placed on a separate area with the counterweight so that smooth handling is available in case of a batching site change. Fuel is transported into the reaction space pneumatically by part of prepared reaction gas, which is supplied from short circuit placed before gas heater. Continuous fuel batching is provided by appropriate vibration of electromagnetic feeder. Fuel sample falls into the stream of transportation reaction gas and carried through water cooled batching unit to the main stream of reaction gas in reaction chamber in the same direction.

Approx. 5 g of a sample is continually batched into the drop tube for 15 minutes long single test period. A small sample quantity and extended batching duration are used in order to avoid substantial reaction of environment conditions by the appropriate power contribution of the fuel reaction.

During “drop” of fuel particles in hot reaction gas towards point of sudden cooling they come to gradual warming-up, drying, releasing and combustion of volatile fraction and then runs burn-out of fixed carbon. During whole process comes to loss of weight which in dependence on time gives burn-out curve in reaction chamber [3]. This process is characterized by kinetic constants that are different for each fuel (as described in the next chapter).

Fig. 1 – Drop tube

At the end of reaction chamber is placed movable sampling device that has especially for this purpose developed nozzle, in which is being injected liquid nitrogen in order to guarantee sudden cooling of hot reaction gas containing sample to the temperature approx. 20 °C. During injection of liquid nitrogen comes up also to inertization of gas and solid particles mixture and ensures quickly and effective quenching to requested temperature. Reacted fuel particles are sampled on ash-less filter (0,007 % ash maximum) with ability to catch particle up to 2.5 μm with diameter of filter of 300 mm (for the purpose of reducing pressure loss during continuous sampling). Mixture of reaction gas and evaporated nitrogen is being sucked off by roots blower. Motor speed and related amount of sucked gas is regulated in dependence of pressure conditions, which occur in reaction chamber in order to keep steady low overpressure in few Pa.

Taken sample is then analyzed, while is determined unburnt fraction U (quantity of unburnt fixed carbon) in dependence of residence time in reaction chamber. These values serve to drawing of burn-out curve that characterizes fuel with given granulometry (particles dimensions) for set conditions, ergo temperature and oxygen concentration in reaction chamber. These results can be also used for setting (specifying) of mathematical model of particles burnout, as described in the next chapter.

2 MATHEMATICAL MODEL OF PULVERIZED COAL PARTICLES BURNOUT IN PROGRAM FLUENT

Movement of solid particles (coal particles) is modeled by multiphase model which is defined by Lagrangian concept. In Lagrangian access gaseous phase is defined as continuous phase. This phase is solved by basic equations for flow of real gases (Navier-Stokes equations, mass conservation equations and energy equation). Second phase consists of spherical particles (which may be taken to represent, droplets or bubbles) dispersed in the continuous phase. Fluent computes the trajectories of these discrete phase entities, as well as heat and mass transfer to/from them. The coupling between the phases and its impact on both the discrete phase trajectories and the continuous phase flow can be included. Then Fluent can include solution of hydrodynamic drag, force of gravity, heating/cooling of the discrete phase, combusting particles, including volatile evolution and char combustion to simulate coal combustion.

Equations of motion for particles solve the trajectory of a discrete phase particle by integrating the force balance on the particle, which is written in a Lagrangian reference frame.

$$\frac{du_P}{dt} = F_D\left(u - u_P\right) + \frac{g_x}{\rho_P}\left(\rho_P - \rho\right) + F_X \tag{1}$$

where:

u – velocity of the gas $\left(m \cdot s^{-1}\right)$,

u_p – velocity of the particle, $\left(m \cdot s^{-1}\right)$,

ρ – density of the gas $\left(kg \cdot m^{-3}\right)$,

ρ_p – density of the particle $\left(kg \cdot m^{-3}\right)$,

g_x – gravity in relevant system of coordinates $\left(m \cdot s^{-2}\right)$,

F_X – additional force $\left(N \cdot kg^{-1}\right)$,

F_D – drag force per unit particle mass $\left(N \cdot kg^{-1}\right)$ and defined as: $F_D = \frac{18\mu}{\rho_P d_P^2}\frac{C_D \,\mathrm{Re}}{24}$

μ – molecular viscosity of the gas $(Pa \cdot s)$,

d_p – particle diameter (m),

Re – Reynolds number $\mathrm{Re} = \dfrac{\rho D_P |u_P - u|}{\mu}$ (1),

C_D – drag coefficient $C_D = a_1 + \dfrac{a_2}{\mathrm{Re}} + \dfrac{a_3}{\mathrm{Re}^2}$, where $a_{1,2,3}$ are constants defined by [4].

In the next step is defined the mathematical model of volatile evolution and char combustion to simulate coal combustion. Program Fluent can define several access of mathematical modeling of these processes.

Process of devolatilization

The devolatilization law is applied to a combusting particle when the temperature of the particle reaches the vaporization temperature T_{vap}. This condition is defined by following relation [5]:

$$T_p \geq T_{vap} \text{ and } m_p \rangle (1 - f_{v,0})(1 - f_{w,0}) m_{p,0} \tag{2}$$

where:

$f_{v,0}$ – fraction of volatiles initially present in the particle (1),

$f_{w,0}$ – mass fraction of the evaporating material (1),

$m_{p,0}$ – initial particle mass (kg),

m_p – particle mass (kg),

The single kinetic rate model

The single kinetic rate devolatilization model assumes that the rate of devolatilization is first-order dependent on the amount of volatiles remaining in the particle

$$-\frac{dm_p}{dt} = k\left[m_p - (1 - f_{v,0})(1 - f_{w,0}) m_{p,0}\right] \tag{3}$$

Note that $f_{v,0}$ the fraction of volatiles in the particle should be defined using a value slightly in excess of that determined by proximate analysis. The kinetic rate k is defined by input of an Arrhenius type pre-exponential factor and activation energy [6]:

$$k = Ae^{-(E_1/RT)} \tag{4}$$

where:

A – pre-exponential factor (1),

E_1 – activation energy $(J / Kmol)$

Process of char combustion (surface combustion)

After the volatile component of the particle is completely evolved, a surface reaction begins which consumes the combustible fraction f_{comb} of the particle until the combustible fraction is consumed.

$$m_p \rangle (1 - f_{v,0} - f_{comb})(1 - f_{w,0}) m_{p,0} \tag{5}$$

where:

f_{comb} – combustible fraction (1)

The kinetic/diffusion surface reaction rate model

The kinetic/diffusion-limited rate model assumes that the surface reaction rate is determined either by kinetics or by a diffusion rate [6]

Diffusion rate coefficient

$$D_0 = C_1 \frac{\left[(T_p + T_\infty)/2\right]^{0.75}}{d_p} \tag{6}$$

and a kinetic rate

$$R = C_2 e^{-(E_2/RT_p)} \tag{7}$$

are weighted to yield a char combustion rate of

$$\frac{dm_p}{dt} = -A_p p_{OX} \frac{D_0 R}{D_0 + R} \tag{8}$$

where:

C_1 – mass diffusion-limited rate constant (1),

C_2 – kinetics-limited rate pre-exponential factor (1),

E_2 – kinetics-limited rate activation energy $(J/kmol)$,

T_∞ – local temperature of oxygen (K),

A_p – surface area of the particle (m^2),

p_{OX} – partial pressure of oxidant species in the gas surrounding the combusting particle (Pa).

Equation 8 is recast in terms of the oxidant mass fraction Y_{OX} as

$$\frac{dm_p}{dt} = -A_p \frac{\rho R T_\infty Y_{OX}}{M_{\omega,OX}} \frac{D_0 R}{D_0 + R} \tag{9}$$

Next mathematical models of devolatilization and char combustion are in detail described in [4].

3 EXPERIMETAL TESTS AND MATHEMATICAL MODELLING OF REAL EXPERIMENTS

Experimental tests were performed with pulverized black coal, which is combusted in Power plant Třebovice. Main properties are in table 1. This coal was sieved with the aim of obtaining granulometry 80-90 μm, it was gained granulometry with Rosin-Rammler index N 1,26 x 39,87 μm.

Tab. 1 Proximate analysis of the coal (as fired)

Proximate analysis (by weight)	
Moisture, $\underline{H^0}$	1.23 %
Ash, $\underline{A^0}$	21.27 %
Volatiles, $\underline{V^0}$	26.27 %
Fixed carbon, $\underline{C^0}$	51.23 %

Tests were performed under various conditions with results as shown in Fig. 3. During two tests temperature of reaction gas was 927 °C, velocity 3 $m.s^{-1}$ and concentration of oxygen 6 $\%_{vol}$ respectively 2 $\%_{vol.}$ In the third case temperature was changed to 1100 °C and oxygen concentration set 6 $\%_{vol.}$ There is very well visible difference between curves in dependence on set parameters in reaction chamber.

These data serve to adjusting of mathematical model of pulverized coal burnout. Model can be set by kinetic constants as narrated in previous chapter. By changing of constants comes up to moving of curves in requested direction with intent to create curve with the shape identical to curve obtained from experimental tests on drop tube. As an example was chosen modelling of burnout under reaction conditions with reaction gas temperature 927 °C, velocity 3 $m.s^{-1}$ and concentration of oxygen 6 $\%_{vol.}$ Figure 4 shows such adjusted curves, which has been set by changing of constants mentioned in table 2.

Tab. 2 Parameters of models

	Default model	Model 2	Model 3	Model 4
A (1)	312 000	312 00	312 00	?
E_1 (J/Kmol)	7.4 e+07	7.4 e+07	7.4 e+07	?
C_1 (1)	5e-12	5e-12	5e-12	?
C_2 (1)	0.002	0.0002	0.00045	?
E_2 (J/Kmol)	7.9e+07	7.9e+07	7.9e+07	?

Default model (single kinetic rate model + the kinetic/diffusion surface reaction rate model) burns out very quickly, while model 2 and 3 differs from default model both devolatilization and fixed carbon burnout. For models 2 and 3 were used the same models of devolatilization and fixed carbon burnout as for default model. It differs only in fixed carbon burnout. Increase of pre-exponential factor by model 3 compared with model 2 brought curve closer to results from drop tube. This method leads to obtaining of appropriate kinetic constants.

In consideration of long computing time, this article contains results which are getting closer to requested shape of curve obtained from real tests.

4 CONCLUSIONS

Contribution describes results from experimental tests which have been carried out with pulverized black coal on new experimental stand built at the Energy Research Center. These data serve to adjusting of mathematical model defined in program Fluent. Mathematical model differentiates devolatilization process from burnout of fixed carbon apparently on course of curves, which can be considerably changed by modification of kinetic constants as pre-exponential factor and activation energy. In the paper are compared varied settings of one mathematical model by modification of these constants. After adjusting of model with data from drop tube, it can be then obtained kinetic constants, which serve to better understanding of burnout process and thus can help with designing of new boilers and consequently increase efficiency of thermo chemical conversion of energy bound in pulverized coal.

REFERENCES

[1] CARPENTER, A., M., SKORUPSKA, N., M., Coal Combustion Analysis and Testing, IEACR/64, IEA Coal Research, London, 1993.

[2] ŽÍDEK, M., HORÁK, J., PALUSKA, R., Experiences with building of drop tube, international conference „Power engineering and environment 2008“, Ostrava, 11th to 12th September 2008, ISBN 978-80-248-1832-0

[3] NOSKIEVIČ, P., OCHODEK, T., PALUSKA, R., MĚCHURA, V., ŠTOSEK, V.: Efektivní metody řešení modernizace kotlů. Článek na konferenci Kotle a energetická zařízení, Brno 2007.

[4] FLUENT: Fluent 6.3.26 - User's guide, Fluent Inc. 2003. VŠB-TU Ostrava. <URL:http://sp1.vsb.cz/DOC/Fluent_6.3.26/html/ug/main_pre.htm>

[5] BAUM, M., M. and STREET, P., J. Predicting the Combustion Behavior of Coal Particles. Combust. Sci. Tech., 3(5):p. 231-243, 1971.

[6] BADZIOCH, S. and HAWKSLEY, P., G., W. Kinetics of Thermal Decomposition of Pulverized Coal Particles. Ind. Eng. Chem. Process Design and Development, p. 521-530, 1970.

[7] M. A. Field. Rate of Combustion of Size-Graded Fractions of Char from a Low Rank Coal between 1200 K and 2000 K. Combustion and Flame, p.237-252, 1969.

Reviewers:

Ing. Pavel Sedláček, Pražská Teplárenská, a.s.
Ing. Petr Matoušů, MORE, s.r.o.

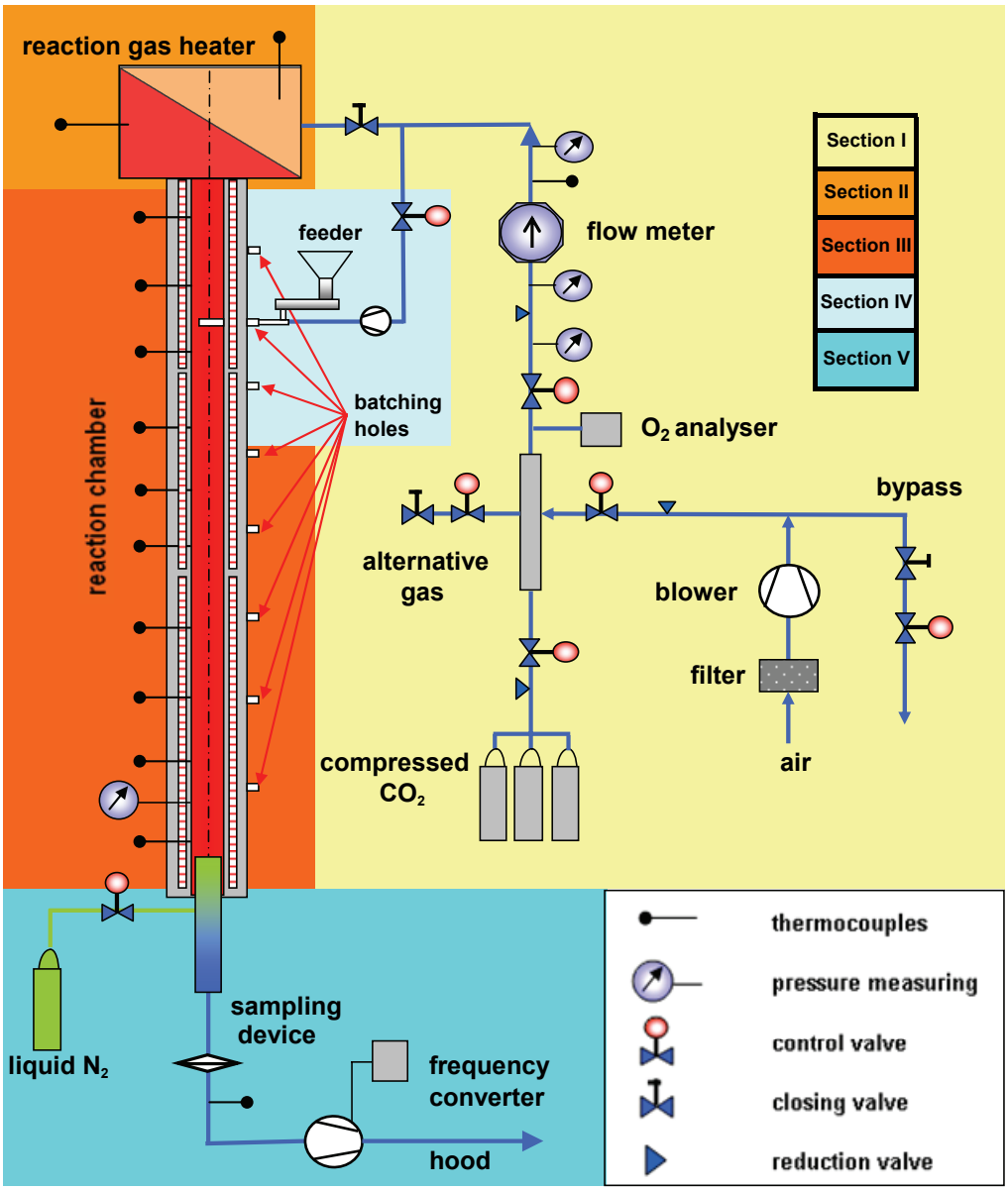

Fig. 2 Simplified layout of the unit

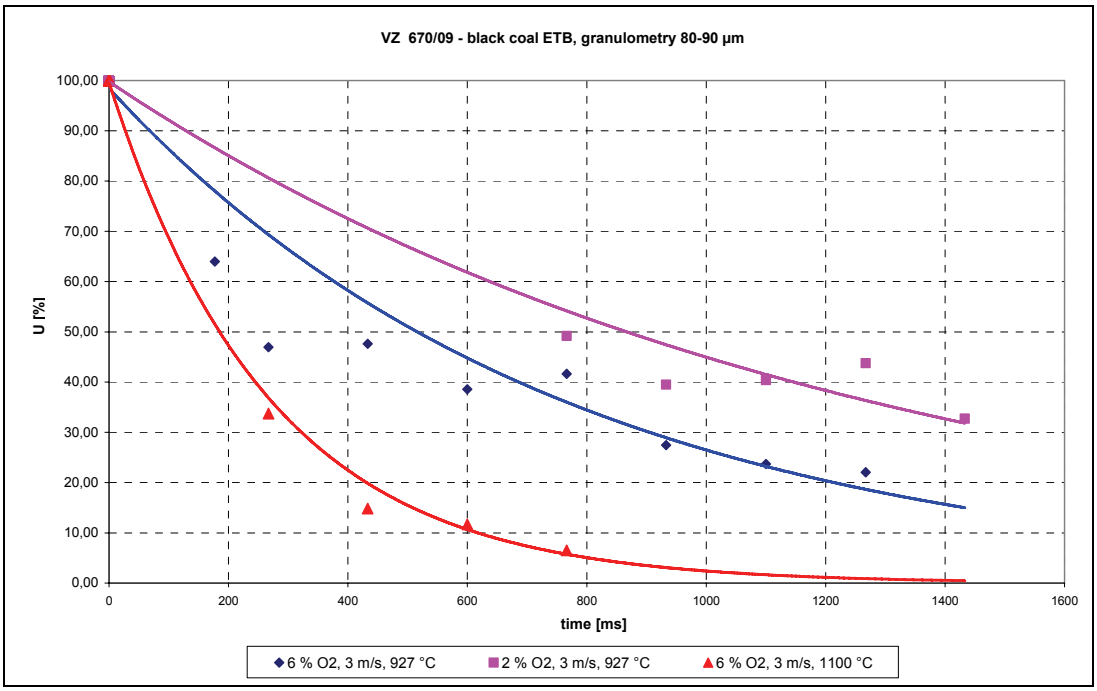

Fig. 3 Unburnt fraction depending on time and set boundary conditions in DTTF with regression curves

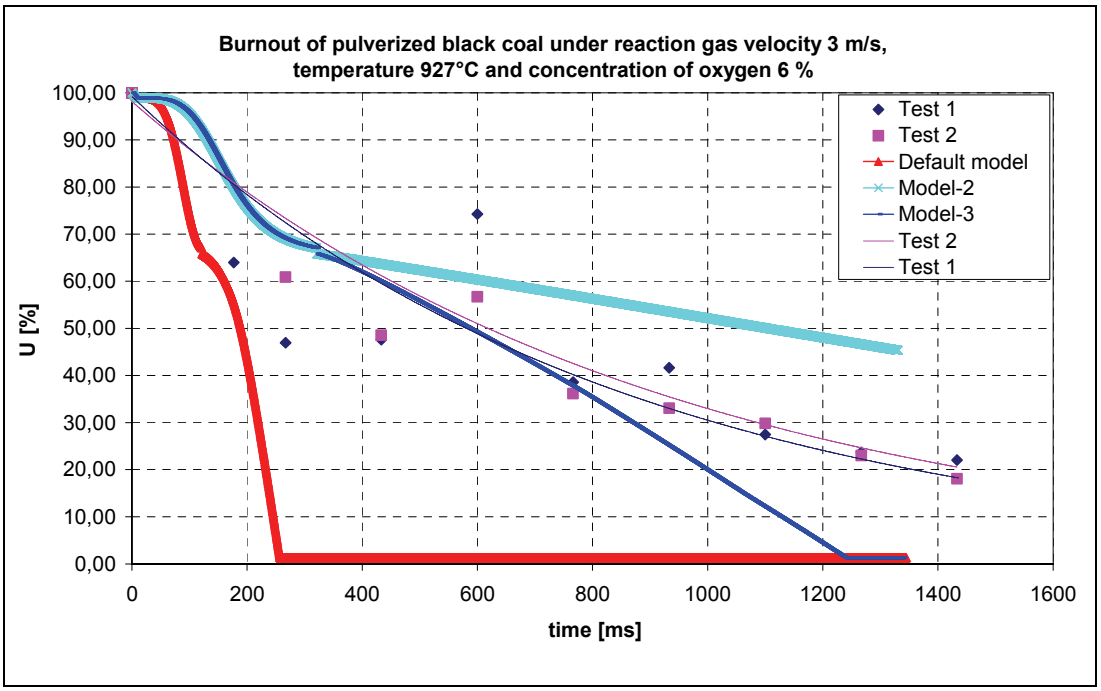

Fig. 4 Example of mathematical models adjusted in dependence on kinetic constants changing