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Performance Devolatilization Model of Lignite during Combustion in PP "Kosova B"

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Abstract: In this paper, a mathematical model for the removal of volatiles from lignite grains is presented. Total amount of volatiles in the dry lignite, experimentally determined, is 44.53%.Such high presence of volatiles makes the lignite reach its ignition temperature very quickly. Methodology of this research is based on laboratory research and the designing of the model for devolution, based on famous equations of different authors, and the programs Microsoft Excel and Mathlab. Results of the simulation are generated for grains with varying activation energy. Distribution function is continuous (E) with f(E)dE which represents the fraction of possible released volatiles $W_{j,\lim}$ with activation energy within E and E+dE.

***Keywords**: Devolatilization model, lignite, global kinetic, activation energy*

Introduction

The dynamic of removal of volatiles from lignite grains is such that when grains begin to heat up, the amount of volatiles in the grains begins to get out of the grains. Volatiles diffuse from the surface of the grains to the surface of the flames, whereas the oxidant diffuses radially from the environment towards the surface of the flames. To model the release of volatiles from lignite grains, modelling is done using the approach that diffusive transfer of oxygen towards the flame surface is unstable, whereas the diffusion of volatiles from inside-out is a process of quasi-steady-state. Via kinetic model it is attempted in the most representative way to show the devolatilization process of lignite in PP "Kosova B" with a general equation such as:

Lignite (dry) $\rightarrow w_v$*(volatiles) + (1-*w_v*) (devolatilizated lignite)*

Materials and Methods

Release rate of volatiles can be calculated using the equation that is similar to that of Arrhenius where the kinetic parameters depend on the type of lignite.

$$\frac{dw_V}{dt} = k\left(w_{V,I} - w_V\right)^n \tag{1}$$

where
$$k_w = k_0 \cdot e^{-\frac{E}{R \cdot T}} \tag{2}$$

and

k_0–preexponential factor, E – activation energy, T–temperature of lignite grain,
w_V–instantenous fraction of volatile substances in lignite,
$w_{V,I}$–total value of volatiles in dry lignite.

Total value of volatiles $w_{V,I}$ and activation energy in dry lignite are experimentally determined (Table 1; Analy Cen&Shërbimii analizave–KEK).

Model for activation energy distribution supposes that devolatilisation occurs via some parallel simultaneous reactions of first order. The method begins with equation (1). Equation (1) now can be written as:

$$\frac{dw_j}{dt} = \sum_i k_i\left(w_{j,\lim} - w_j\right) \tag{3}$$

Index j can represent not only gas products but also fluids and solids that are treated during devolatilisation. The special entity j can be treated from one or more reactions i. Assumptions for the

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*Corresponding: E-Mail: ismet.mulliqi@umib.net; Tel: +377(0)44176310 reaction of first order allow the simplification and regulation of equation (3), by writing:

$$k_j = \sum_i k_i \tag{4}$$

where the summation should be performed only for the reactions of first order in which entities *j* are included.

Table 1.Analysis of lignite that is used for combustion in the boilers of PP “Kosova B”

Summary of analysis	Mean	Maximum	Minimum	Unit
Moisture	42.46	47.1	33.8	*%*
Ash	33.06	44.7	20.2	*%*
Ash (in the used sample)	19.23	28.7	10.9	*%*
Volatiles	44.53	51.1	36.8	*%*
Volatiles (in the used sample)	25.52	28	21.2	*%*
C-fix	22.42	28.7	15.3	*%*
C-fix (in the used sample)	12.79	16.1	9.3	*%*
Sulphur S	1.98	3.07	1.1	*%*
Sulphur S (in the used sample)	1.15	1.98	0.65	*%*
Sulphur S (inorganic)	3.64	5.21	1.58	*%*
Chlorine Cl	<0.01	<0.01	<0.01	*%*
Chlorine Cl (in the used sample)	<0.01	<0.01	<0.01	*%*
Carbon C	42.30	50.7	34.9	*%*
Carbon C (in the used sample)	24.22	27.3	20.2	*%*
Hydrogen H	3.11	3.8	2.7	*%*
Hydrogen H (in the used sample)	6.54	7.2	5.7	*%*
Nitrogen N	0.86	1.3	0.66	*%*
Nitrogen N (in the used sample)	0.49	0.75	0.4	*%*
Oxygen O	18.68	22.7	14.3	*%*
Oxygen O (in the used sample)	48.37	53.4	39.8	*%*
Fluorine F (in the used sample)	63.25	125	33	*mg/kg*
Energetic value	16.19	19.54	13.49	*MJ/kg*
Energetic value(in the used sample)	9.27	10.55	7.99	*MJ/kg*
Activation energy	94.6	96.8	92.4	*KJ/mol*
Emission factor (calculated)	99.86	103	96.9	$t/TJ\ CO_2$
Deformation temperature	1223	1280	1180	*°C*
Flow temperature	1273	1360	1200	*°C*

Integration of equation (3) gives us:

$$w_j = w_{j,\lim}\left[1 - \exp\left(-\int_0^t k_j\,dt\right)\right] \tag{5}$$

If the Arhenius equation is also used for the kinetic, then:

$$k_j = \sum_i k_{0,i}\exp\left(-\frac{E_i}{RT}\right) \tag{6}$$

For isothermic conditions, equation (5) can be written in the form:

$$w_j = w_{j,\lim}\left\{1 - \exp\left[-\sum_i k_{0,i}\,t\exp\left(-\frac{E_i}{RT}\right)\right]\right\} \tag{7}$$

As it can be seen, this expression includes all of the pre-exponential coefficients $k_{0,i}$ and activation energy E_i. Method of activation energy distribution includes the following simplifications (Pitt, 1962):

- All the pre-exponential coefficients are equal, so$k_{0,j}=k_0$.
- The number of reactions is considerable and makes it possible to express activation energy as a continuous function of distribution *f(E)* with *f(E)dE* that represents the fraction of possible

released volatiles $w_{j,lim}$, and that becomes a differential part of the total loss of volatiles and it can be written as:

$$dw_{V,\lim} = w_{V,\lim} f(E)dE \tag{8}$$

with

$$\int_0^{\infty} f(E)dE = 1 \tag{9}$$

Using equations (1-9), the total value of released volatiles in isothermic conditions can be written, from $t=0$ to a specific time t as:

$$w_V = w_{V,\lim}\left\{1 - \int_0^{\infty} \exp\left[-k_0 t \exp\left(-\frac{E}{RT}\right)\right] f(E)dE\right\} \tag{10}$$

After we have chosen the correct distribution function, the value of pre-exponential factor $k_0$can be found by adjusting the theoretical and experimental curves of released volatiles. The main problem of this method is the assumption that the devolatilization process, from the beginning until the very end, takes place under isothermal conditions. Other authors (Anthony & Howard, 1976; Arenillas *et al.*, 2001)generalised explanations of Pittand by using the general equation (9) they found the expression that determines the total value of volatiles even for non-isothermal conditions from the begging of the process ($t=0$) to a time t:

$$w_V = w_{V,\lim}\left[1 - \int_0^{\infty} \exp\left(-\int_0^{t} f(E)dE\right)\right] \tag{11}$$

Then they supposed that we have to do with the function *f(E)*,with the Gauss distribution with average activation energy and with standard deviation σ_V. Thus this equation follows,

$$f(E) = \left[\sigma_V (2\pi)^{1/2}\right]^{-1} \exp\left[-(E-E_0)^2 / 2\sigma_V^2\right] \tag{12}$$

Results and Discussions

Values of the parameter σ_V= 18.5*KJ/mol* and the preexponential coefficient k_0=15.4s^{-1} are obtained from the adjustment of curves for the released volatiles. Solution of equation (1), for the reaction of order n =3, brings the functional relation (13) between the release time and release rate of volatiles that is shown in table 2, and in figure 3 respectively.

$$t = \frac{1}{2 \cdot k_0 e^{-\frac{E}{RT}}} \cdot \frac{1}{\left(w_{V,I} - w_V\right)^2} \tag{13}$$

where: $w_{v,I}-w_v=w_j$ (14)

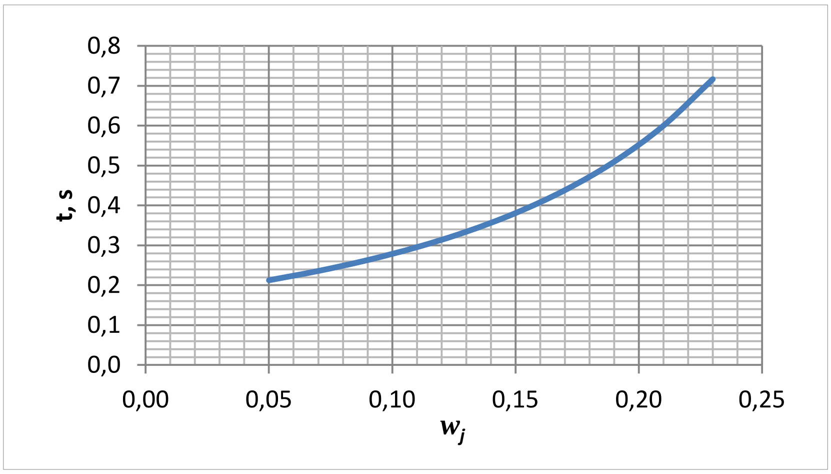

Figure 1. Dependence between release rate and release time of volatiles from lignite

Table 2. Simulation of time-dependent release of volatiles from lignite

R*=8.314*KJ/mol*; *n*=3; *ko*= 15.4s^{-1}; *E*=94.6*KJ/mol*; $w_{V,I}$=44.53%; *T*=1000*K										
w_j	0.050	0.070	0.090	0.110	0.130	0.150	0.170	0.190	0.210	0.230
t,s	0.213	0.236	0.263	0.295	0.334	0.381	0.438	0.510	0.600	0.717

Dependence of the coefficient of volatiles release kinetics from temperature and activation energy according to equation (2) is shown in the Figure 2:

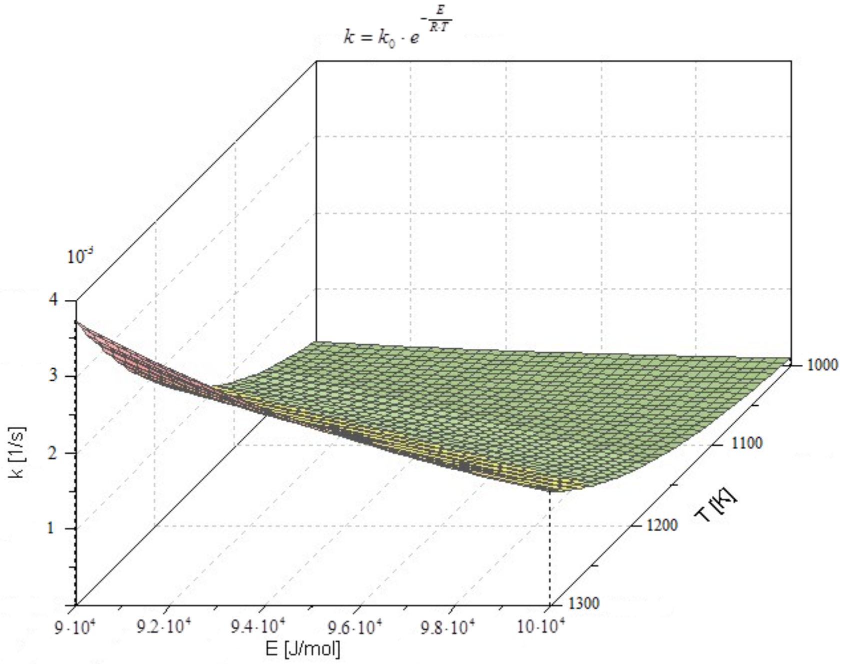

Figure 2. Dependence of the coefficient of volatiles release kinetics from temperature and activation energy

Results of the simulation for dovolatilization of lignite that is burned in the boilers of PP "Kosova B" are generated for grains with varying activation energy. Results mainly suggest that the distribution function is continuous *f(E)with f(E)dE*,and represents the fraction of possible released volatiles with activation energy within *E* and*E+dE*, that in accordance with equation (12), the graphical representation of the function is shown in the figure 3.

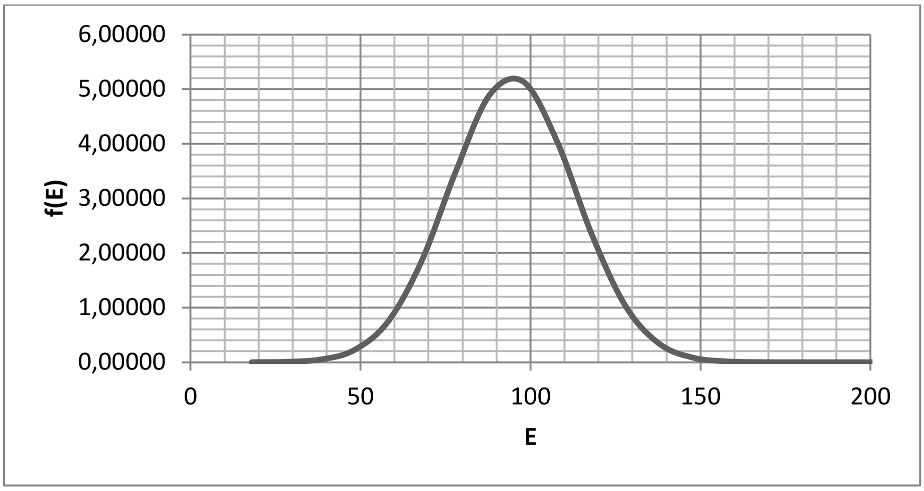

Figure 3. Normal distribution function of activation energy

Conclusions

- Predictions of the model show that presence of higher values of the amount of volatiles in the grain increases the chance for lignite to ignite easier.

- For 0.3*s*, 11.5*%* of volatiles are released from lignite grains, whereas for 0.7*s*,23*%* of volatiles are released from the total amount of volatiles.
- Distribution function is continous *f(E)* with *f(E)dE* which represents the fraction of possible released volatiles $W_{j,lim}$ with activation energy within *E* and *E+dE*.
- Model for describing the release of volatiles from the lignite grains gives a good explanation of the dynamics of the process.
- Regardless of the good predictions for the release rate of volatiles, there are no good predictions for the release of specific types of volatiles.

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