

NEW APPROACH TO APPLICATION OF CLASSIC METHODS OF PHYSICAL AND CHEMICAL KINETICS TO ANALYSIS OF EFFICIENCY OF PLASMA TECHNOLOGY OF COAL GASIFICATION

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ABSTRACT

This report is devoted to the problem of increase of the efficiency of new plasma technology of coal burning providing minimum negative influence to the environment [1, 2]. In particular, common method of statement and solution of inverse kinetic problem allowing to show plasma gasification advantages is represented here.

I. INTRODUCTION

At present the conventional methods of analysis of kinetics problems in all modifications are based on total consideration of physical and chemical processes including stage by stage conversion of most reaction components taking into account their specific characteristics. In this case the equations of heat and mass transfer for interacting masses – heating, diffusion for coal particles and plasma processes and hydrodynamic characteristics of given reactor defining the track and velocities of coal particles are considered jointly. In the terms of mathematics these statements lead to the necessity of joint solving of very large systems of quite approximate differential equations (more than hundred equations) with numerous parameters which are known to be poorly conditioned. This gives no hope to obtain real satisfactory results, however, the study of this field is slightly progressing. These methods are called "differential" due to the necessity of consideration of many physical and chemical processes with regard to the specific characteristics and consequent summation.

However, another approach is valid. It is called "integral" because it includes (at least on the first stage) direct consideration of general effects from all above mentioned factors influencing on kinetics. It becomes possible if we go to the probability method and accept generalized kinetic Erofeev's equation [3] which is in fact equivalent to the set of classical kinetics equations. In this case the deciding factor is the introduction of the concept of reaction probability at given time of reagent residence in the reaction zone.

II. THEORETICAL BASIS AND RESULTS

Our approach is based on two formulas: Erofeev's formula (1) for reaction probability and our formula (2) that includes the characteristics of reagent residence in the reactor:

$$\alpha = 1 - \exp\left(-\int_0^{\tau} p(\tau) d\tau\right), \quad \text{or} \quad \alpha'(\tau) = (1 - \alpha)p(\tau), \quad (1)$$

where $\alpha(\tau)$ – the part of reacted substance (in relation to the amount of initial substance). We assume that the substance reacts continuously during the time period τ , $p(\tau)$ – reaction probability by the time of τ .

$$D(T) = \frac{1}{T} \int_0^T \int_0^{T-\tau} y(\tau) \alpha'(\tau) d\tau d\tau = \frac{1}{T} \int_0^T \int_0^{T-\tau} y(\tau) e^{-\int_0^{\tau} p(\tau) d\tau} p(\tau) \tau d\tau, \quad (2)$$

where $D(T)$ – the part of the substance entered the reactor (in relation to initial amount) reacted during the apparatus operation, $y(\tau)$ – the part of reagent flow entered the reactor that spends in reactor no less than time τ ; $\alpha'(\tau)$ – the value from formula (1).

The formula (2) connected the Erofeev's equation with characteristic of reagent residence in reactor $y(t)$ is obtained by tracing of the passage of elementary part of reagent flow through the reactor during the time period $(0, T)$. In this case, double integral sum going over in the limit to double integral of formula (2) has been obtained.

Usual and quite simple diffusive or cell model of mixing process in reactor is easy identified by experimental data of dynamics, and then $y(\tau)$ is obtained. In particular, we used diffusive one-parameter model. It should be noted that when constructing the solution and identifying the diffusive and cell models it is rationally to use the method of moments leading to simple analytical solutions [4, 5, 7].

Technical realization of necessary dynamic experiments defining $D(\tau)$ and $y(\tau)$ is simple and doesn't require special explanations. It should be only noted that when stationary work regime of the system is reached a disturbance defined by uranium presence at the reactor entry is introduced over coal dust in the form of pulses mentioned above (coal contaminated by uranium). When disturbance is introduced the extraction of slag into cylindrical glass long enough to cover all transient regime begins simultaneously at the reactor outlet. Then the fibered analysis of various chemical transformations (carbon burn-out, output of volatile components etc.) was made in selected probes. Also, in this probes the uranium percentage was defined by laser method. Using one-parameter model, we define the characteristics of mixing.

The equation (2) for homogeneous and heterogeneous processes in reactors as well as Erofeev's equation is obtained without differential equations based on the laws of interacting masses. Besides, while deriving this equation no specific assumptions

concerned with the properties of reacting system were used. Thus, we can't work out details of transient reactions and consider only the final results. The inverse kinetic problems of coal gasification will be solved by this equation.

As a result using the integral equation obtained with the help of generalized equation of physical and chemical kinetics at the statement and solution of inverse problem, we show the integral effect of significant increase of reaction probability in plasma reactors. The substantial increase of reaction probability for plasma reactors in comparison to other devices is caused by following feature of low temperature plasma. At relatively low mass average temperature plasma contains large number of active centers favoring rapid development of reaction processes.

Simple and well known approximation of the function $y(\tau)$ is used for accepted mathematical model of mixing in the reactor with the help of inertial component of the first order and dead time. Thus we obtain the characteristic of residence time in the form of

$$y(t) = \begin{cases} 1, & \tau \leq \tau_0, \\ e^{-\frac{\tau-\tau_0}{m_1}}, & \tau > \tau_0, \end{cases} \quad (3)$$

where τ_0 – dead time, m_1 – the constant of the time of inertial component which is equal to its power moment of the first order.

Taking into account (3) we split the time interval $(0, T)$ for $D(T)$ into two parts and obtain $D = D_1 + D_2$.

$$D_1(\tau_0) = \frac{1}{\tau_0} \int_0^{\tau_0} \int_0^{\tau_0-\tau} \alpha'(\tau) d\tau d\tau = 1 - \frac{1}{\tau_0} \int_0^{\tau_0} \exp\left(-\int_0^{\tau} p(\tau) d\tau\right) d\tau, \quad (4)$$

$$D_2(T_1) = \frac{1}{T_1} \int_0^{T_1} \int_0^{T_1-z} \exp\left(-\frac{z}{m_1} - \int_0^z p(z) dz\right) p(z) dz dz, \quad T_1 = T - \tau_0. \quad (5)$$

It is known that at the velocities of coal particles heating in plasma and usual sizes of the particles the rejection of volatile components comes about as the reaction of the first order [6]. Therefore, we consider the reaction of the first order as an example. In this case $p = K = \text{const}$. Substituting $p = K$ into (4, 5) we obtain

$$D_1 = 1 - \frac{1}{\tau_0} \int_0^{\tau_0} \exp\left(-\int_0^{\tau} K d\tau\right) d\tau = 1 - \frac{1 - \exp(-K\tau_0)}{K\tau_0}, \quad (6)$$

$$D_2 = \frac{Km_1}{1+K_1} - \frac{K^2 m_1^2}{T_1 K (1+Km_1)^2} \left(1 - e^{-\frac{T_1 - K T_1}{m_1}}\right). \quad (7)$$

Proposed simple model (6, 7) is very practical and may be recommended for engineering technological calculations. It integrally takes account of two main factors that are present in all real characteristics of reactor: the factors of direct displacement and mixing.

Based on experimental data obtained the calculations of reaction probabilities for stationary regime in plasma and usual thermal reactors have been carried out. For example, during the experiments with usual thermal heating the reaction probability of volatile components output at the mass average temperature of 853 K was equal to $p_{\beta_1} = 0.108$. During the experiments in electric arc plasma at the same mass average temperature and the same coal consumption (1.4 kg/h) reaction probability was equal to $p_{\beta_2} = 0.240$, i.e. it increased more than twice. In all cases at different methods of carrying out the process the condition of equal consumptions of energy on reactor operating was satisfied.

Resulted from the processing of the same experimental data and computations of reaction probability over carbon combustion the following inferences are made. For the condition of ordinary thermal heating $p_{\alpha_1} = 0.072$, and with electrical arc heating $p_{\alpha_2} = 0.198$. Thus, the reaction probability increased in 2.7 times as much. A series of other experiments showed the analogous effect of the severe increase. To take into account the influence of plasma state of reactor environment to kinetics additional parameter $\gamma < 1$ correcting the decrease of activation energy E has been entered into Arrhenius equation for velocity constant $K = K_0 \exp(\gamma E/RT)$, where R – gas constant, T – absolute temperature.

In accordance with this method of calculations using the same experimental data as that the reaction probability was defined by the values of activation energy under usual (thermal) heating and under plasma heating were calculated. In the first case for volatile components output $E_{\beta_1} = 151.242$ J/mol, in the second case $E_{\beta_2} = 23.902$ J/mol, i.e. activation energy when plasma is used is 6 times less than in the first case.

For the same experiments but over carbon combustion resulted from the computations with the same technique we obtained $E_{\alpha_1} = 285.048$ J/mol, $E_{\alpha_2} = 53.780$ J/mol. So, the activation energy diminished in more than five times.

Activation energy E even for the process with merely thermal activation obtained under laboratory conditions is noted to differ from that obtained on the reactor itself where there are some features of reaction zone, design of reactor and burner and others.

Therefore, for the design with non-thermal activation this difference is likely to be larger. Thus, after graduation of the activation energy over coal it is necessary to generally correct their values (to diminish or increase) for given designs of reactors (on the basis of experimental data).

Virtually, the data of activation energy for plasma technology can be. In conclusion it may be said that new approach to the analysis of physical and chemical kinetics based on generalized probability characteristics of heterogeneous processes in reactors allows to carry out an integral estimation of the factors influenced on plasma technology efficiency. In particular, when the most important factor – the time of residence is

analyzed, the method integrally takes into account the aerodynamics influence and the concept of reaction probability includes the constant of reaction rate.

As a result analytical solutions allowing to indicate and explain physical and chemical essence of plasma technology advantages concerned with increase the energy of processes activation are obtained.

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