Modeling of mechanism of obtaining mesostructural coal matrix in pyrolysis processes.

Valeriy Kotelnikov (✉ tikopr@mail.ru)

Novosibirsk institute of organic chemistry Siberian Branch of Russian academy of sci.

<https://orcid.org/0000-0001-7481-9770>

Elena Ryazanova

Tuvanian institute of Exploration of natural resources Siberian Branch Russian academy of sci.

Olesya Ershova

Institute of archeology and ethnography Siberian Branch of Russian academy of sci.

Short Report

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Abstract

Reducing the role of coal in the energy balance of countries and the whole world sets the task of improving coal combustion technologies and creating new environmentally friendly processes for deep processing of coal. The production of high-quality raw materials for the metallurgical industry and other industries is a strategic task for the development of the country. In this study we try to use an Monte Carlo method to analyze and modeling of coke producing process in the device for continuous pyrolysis of organic materials in a thermally loaded layer.

1. Introduction

Reducing the role of coal in the energy balance of countries and the whole world sets the task of improving coal combustion technologies and creating new environmentally friendly processes for deep processing of coal. The production of high-quality raw materials for the metallurgical industry and other industries is a strategic task for the development of the country. To replace the retired coal deposits, it is necessary to put into operation new deposits. However, this process is rather complicated, since the coals of different deposits differ in composition and properties and, accordingly, the cokes obtained from such coals differ in quality and physical parameters. In this regard, there is no single technological process for all coal deposits and there is a need to adapt the technology in accordance with the change in the properties of the coals used, especially when moving to deposits in different regions of the country. On the other hand, in the light of the latest decisions of the leadership of the Russian Federation, it is necessary to solve the assigned tasks within the framework of energy efficiency and economic feasibility.

Currently, there are no implemented developments of environmentally friendly energy-saving technologies for burning solid fuels based on coals from the region. The main use of coal is for power generation; preliminary technological processing of coal is not applied. Due to the high content of "volatiles" and the tendency to sintering, layered combustion of coals in boilers and household furnaces is accompanied by high chemical underburning, which leads to severe pollution of the atmospheric air with products of incomplete combustion of coal.

2. Results And Discussion

The intensity of gas evolution during pyrolysis of G grade coal particles is 2-3 times higher than that of T or CC grade coal particles. At high velocities of pyrolysis gases and the presence of small particles in the fuel, they are picked up by the flow of gases and removed from the working space of the furnace. In addition, volatile products emitted from coals with sintering properties are characterized by a high content of hydrocarbon components that decompose with the formation of low-reaction soot, which does not have time to burn and is also carried out from the working space of the furnace. When particles of G grade coal were ignited, an explosive nature of the process was observed with scattering of gas jets, solid

and liquid emissions. The technology makes it possible to obtain carbon material with unique properties (Table 1.)

Nº	Parametr	Value
1.	Ash content, %, no more	15
2.	Mass fraction of sulfur, %, no more	0,6
3.	heating value, kkal/kg, not less	5500
4.	Resistivity, Ohm	40
5.	quantity mesopores	>50

To analyze the data obtained and verify the above assumptions, a mathematical model was developed for the alleged process of the formation of a carbon matrix (Monte Carlo method). The change in the structure of the matrix under the influence of high temperature and pressure was simulated.

Figure 3 shows that the quantity of pores at the beginning of the process go up. Then, apparently, an equilibrium occurs between the detached carbon particles under the influence of temperature and the precipitation of C-C fragments contained in the gas phase. We can change the pressure and temperature programmatically and investigate the pyrolysis process in various combinations of parameters.

The red line on the graph, the virtual weight loss of the sample, coincides with the experimentally found on the STA 449 Netzsch (Fig. 4). The growing interest in coking coals due to their high qualities, such as low sulfur content, high vitrinite content, low ash content, stimulates the search for new innovative methods of using coal. Coal is a complex organomineral substance, and therefore has a variety of useful properties. This predetermines the possibility of its use in almost all sectors of the economy - from an elementary household stove to spacecrafts.

As a first approximation, the following reaction kinetics can be assumed:

CO₂ is produced in an amount that corresponds to the amount of oxygen in the system. The pyrolysis process stops most likely when most of the carbon goes into an elemental state (semi-coke-coke-graphite).

Based on the above equations, an algorithm for the model of the pyrolysis process in the VS Microsoft environment was implemented. The model is a software module with a Windows.Forms graphical interface, with the ability to change the program parameters that simulate the parameters of the pyrolysis process. The appearance of the software interface is shown in Fig. 5.

3. Conclusion

The developed module can be used to conduct virtual experiments during the period of restrictions due to the spread of COVID-19. The module is designed to simulate the technology of continuous supercritical pyrolysis of coal. A feature of this technology is the pyrolysis process under supercritical conditions. When heating the mass of prepared coal entering the installation, an intensive release of volatile coal and organic substances of complex composition obtained during heating occurs. Released substances act on coal under conditions of supercritical states of the components, washing out soluble organic components from the solid part of the coal, as a result of which it is possible to create conditions for the directed carrying out of reactions of transformation of the initial coal in the required direction and obtaining high-quality materials and products.

Declarations

Competing interests: The authors declare no competing interests.

References

1. Ruihan Wang, Qiang Wang, Zhuangmei Li, Zhe Liu, Yong Wu, Jinpeng Zhang, Hongcun Bai, Qingjie Guo. Pyrolysis Reactive Behaviors and Kinetic Characteristics of HSW Vitrinite Coal based on Coats-Redfern and DAEM Models. <https://doi.org/10.21203/rs.3.rs-389404/v1>. 2021.
2. Yan J C, Liu M X, Feng Z H, Bai Z Q, Shui H F, Li Z K, Lei Z P, Wang Z C, Ren S B, Kang S G, Yan H L. Study on the pyrolysis kinetics of low-medium rank coals with distributed activation energy model[J]. Fuel,2020,261:116359.
3. Xu J J, Zuo H B, Wang G W, Zhang J L, Guo K,Wang L. Gasification mechanism and kinetics analysis of coke using distributed activation energy model (DAEM)[J]. Applied Thermal Engineering,2019,152:605-614.
4. Zou C, Ma C, Zhao J,et al.Characterization and non-isothermal kinetics of Shenmu bituminous coal devolatilization by TG-MS[J].Journal of analytical and applied pyrolysis, 2017, 127: 309-320.
5. Solomon P R, Serio M A. Cross-link reaction during coal conversion [J].Energy Fuels, 1990,4,42.

6. Bemgba Bevan Nyakuma, Aliyu Jauro, Segun Ajayi Akinyemi, Hasan Mohd Faizal, Mohammed Baba Nasirudeen, Muhammad Ariff Hanaffi Mohd Fuad, Olagoke Oladokun. Physicochemical, Mineralogy, and Thermo-Kinetic Characterisation of Newly Discovered Nigerian Coals under Pyrolysis and Combustion Conditions. 10.21203/rs.3.rs-34191/v3
7. Ahmed I. Osman, Charlie Farrell, Ala'a H. Al-Muhtaseb, Ahmed S. Al-Fatesh, John Harrison, David W. Rooney. Pyrolysis kinetic modelling of abundant plastic waste (PET) and in-situ emissions monitoring. Environmental Sciences Europe volume 32, Article number: 112 (2020).
8. M. Wagner, M. Engwall, H. Hollert, Editorial: (Micro)Plastics and the environment, Environmental Sciences Europe, 26 (2014) 16.
9. N. Beagan, K.E. O'Connor, I.J. Del Val, Model-based operational optimisation of a microbial bioprocess converting terephthalic acid to biomass, Biochemical Engineering Journal, 158 (2020) 107576.
10. Ruktai Prurapark, Kittwat Owjaraen, Bordin Saengphrom, Inpitcha Limthongtip, Nopparat Tongam, Effect of Temperature on Pyrolysis Oil Using HDPE and PET Sources from Mobile Pyrolysis Plant. 10.21203/rs.3.rs-24640/v1
11. Binay Kumar Samanta, Dharavath Ramesh, Multi-Project Model Program Runs With Algorithms to Improve Indian Coal Mining. 10.21203/rs.3.rs-130977/v1.

Figures

Figure 1

The microstructure of the carbon matrix wall. Overgrowing pore.

Figure 2

Program execution results modeling the pyrolysis process. White - pores, red re-settled carbon particles, black - original coal

Figure 3

Mass loss graph (red) and the number of pores (blue).

Figure 4

STA diagram of coal pyrolysis.

Figure 5

User interface of the pyrolysis process simulation program.

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