

*Матеріали Міжнародної науково-технічної конференції 14–15 травня 2020 року
«Фундаментальні та прикладні проблеми сучасних технологій», Тернопіль, Україна*

UDC 669.046:536.24.001.57

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COMPACTING CARBON COMPOSITES BY PRODUCTS PYROLYSIS OF NATURAL GAS IN THE THERMOCHEMICAL FLOW-TYPE REACTORS

At the production of carbon composites one of the important stages is a compacting of their porous structure by pyrocarbon from a gas phase with the use of natural gas (methane). During of homogeneous reactions, in the thermochemical flow-type reactors the complex of saturated and unmaximum hydrocarbons, and also row of radicals appear. Initial hydrocarbon and products of homogeneous reactions diffuse to the heated surfaces of composite and into its porous structure with subsequent decomposition on the heated walls of pores and formation of solid phase, namely pyrocarbon.

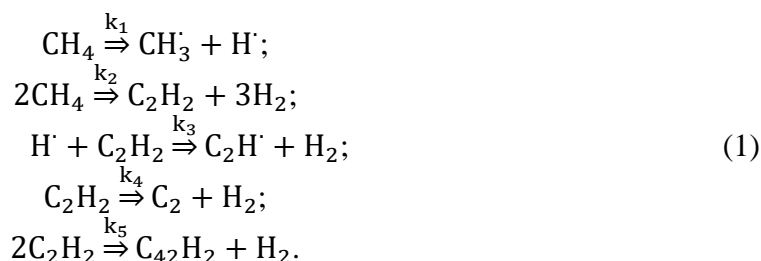
Equations of mass transfer for components of reaction gas mixture and chemical transformation are offered in the conditions of gas flow along the axis of reactor. A correlation of the concentration of components of reaction gas mixture in the volume of reactor and on the surface of porous composite is obtained, which was specified by the twostream approaching for porous bodies.

At solving the system of equations of mass transfer for components of reaction gas mixture the circular axisymmetrical reactor was considered, for which the function describing the structure of gas streams, does not depend on a circuitous coordinate, and office hours is stationary. Also, it was supposed that deposition rate of pyrocarbon in the porous structure of composite was low enough, and porosity of composite is the slowly changing function of time. For this case, a task about the mass transfer in the single cylindrical pore in carbon composite was formulated and the transcendent equation of the change of density of composite material on the thickness of its wall was obtained.

Introduction

Target-setting. At the production of carbon composites one of the important stages is a compacting their porous structure by pyrocarbon with the use of natural gas (methane) [1]. When homogeneous reactions occur, the complex of paraffinic and unsaturated hydrocarbons and a number of radicals appears [2-5]. Products of homogeneous reactions and initial hydrocarbon diffuse to the heated surfaces of composite and then into its porous structure where subsequently decomposition on heated walls of pores and form a solid phase, namely pyrocarbon.

The assemblage of volume chemical reactions of methane pyrolysis can be presented as system of equations:



Carbon composite samples and reactor walls have almost identical temperatures. Near the heated surfaces of composites, the temperature of reaction gases corresponds the temperature of reactor walls, but with distance from walls the temperature of gases decreases and in area of mainlines of its flow has a minimum value.

Objective of the work is to study the processes of mass transfer of reaction gases mixture and deposition of pyrocarbon in flow-type reactors at the compacting of carbon composite from a gas phase.

For conditions of gas flowing along the reactor axis and diffusion rate lower than flow rate, equations of mass transfer of i -th component of reaction gas mixture and chemical transformation can be written as:

$$\frac{\partial C_i}{\partial \tau} = \operatorname{div}(\bar{V} \cdot C_i - D_{iN} \cdot \Delta C_i) = k_i \cdot C_1^n \cdot C_2^n \dots C_N^n, \quad (2)$$

where C_i – a concentration of i -th component of gas mixture; D_{in} – a coefficient of diffusion of i -th component from mixture of N components; ΔC_i – a concentration gradient; k_i , n – a rate constant of homogeneous reaction and reaction order on i -th component respectively.

A solving of the system of equations (2) is possible, if the initial and border conditions of the studied process are known.

Computing experiment with the use of the offered mathematical model was performed by means of the computer program in programming environment «Delphi».

Initial data for the calculation are natural gas composition and flow rate; geometrical parameters of reactor; initial porosity and thickness of carbon composite wall; middle radius of pores; temperature and remaining pressure in reactor; duration of pyrocarbon deposition process.

The out parameters are distribution of individual hydrocarbons (radicals) concentration in the volume of reactor and in the porous structure of carbon composite; deposition rate of pyrocarbon; distribution of composite density on the wall thickness for its different areas.

As a numeral example the calculation of pyrolytic compaction of composite was executed for next conditions: composite on basis of graphitized carbon clothes with novolak-type binder; natural gas (96,50 % CH_4 ; 0,54 %; C_3H_8 ; 0,44 % C_2H_6 ; 0,20 % C_4H_{10} ; 1,5 % H_2 ; 0,82 % N_2) at a temperature 1050-1100 °C; remaining pressure 1.0 kPa, open porosity of composite - 24 %; middle radius of pores 7,0 μm).

Authentication of the offered mathematical model was performed by comparison of calculated values of carbon composite density with real ones obtained during in optical and mechanical researches. It was found that variance of theoretical and experimental values of density is, on average 0.5 %, that confirm to applicability of the offered model to the quantitative estimation of density distribution on thickness of composite wall at its compacting from a gas phase.

The model for natural gas pyrolysis process and mass transfer of reaction gas mixture at compacting of carbon composites by pyrocarbon deposited in flow-type reactor is developed. Offered model was successfully tested at practical calculations of pyrolytic compacting carbon composites` in reactors of different construction.

References

1. Tesner, P.A. (1972). *Образование угля из газовой фазы* [Formation of carbon from gas phase]. Moskva : Khimiia [in Russian].
2. Poltorak, V.A., & Voevodskii, V.V. (1954). *O edinom tsepnom mekhanizme termicheskogo raspada uhlevodorodov* [About the single mechanism of thermal decomposition of hydrocarbons]. *Doklady AN SSSR – Lektors of AS the USSR*, Vol. 91, 3, 589-591 [in Russian].
3. Maharil, R.Z. (1973). *Образование угля при термических превращениях индивидуальных углеводородов и нефтепродуктов* [Formation of carbon at thermal transformations of individual hydrocarbons and petroleum products]. Moskva : Nauka [in Russian].
4. Makarov, K.I., & Pechik V.K. (1975). *Issledovanie kinetiki termoklimicheskogo prevrashcheniia metana* [Research of kinetics of thermal transformation of methane]. *Kinetika i kataliz – Kinetics and Catalysis*, XVI, Vol. 6, 1484-1500 [in Russian].
5. Deriahin, B.V., & Fedoseev, D.V. (1977). *Rost almaza i hrafita iz gazovoi fazy* [Growth of diamond and graphite from a gas phase]. Moskva : Nauka [in Russian].