On a method of mathematical modeling of the pyrolysis process to produce nanomaterials from natural gas

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Abstract: In this paper we developed a method for implementing a mathematical model of the methane catalytic pyrolysis to produce nanomaterials in periodic and continuous mode. It is shown that the Laplace transform method is mostly appropriate for this case, which is applicable both for the differential equations for the solid-phase components and for calculating the periodic mode. The adequacy of the resulting solution with known experimental data has been checked. Mathematic formulation is of the following mode [**?**]:

$$\frac{\int \partial C_i}{\partial t} + v_1 \frac{\partial C_i}{\partial x} = D_i \frac{\partial^2 C_i}{\partial x^2} + D_i \frac{\partial^2 C_i}{\partial r^2} + \frac{D_i}{r} \frac{\partial C_i}{\partial r} + \alpha_{i-1} C_{i-1} + \beta_{i+1} C_{i+1} + J_i,$$

$$C_i(t = 0, x, r) = C_i^0(x, r),$$

$$C_i(t = 0, x, r) = C_i^L(r),$$

$$\frac{\partial C_i}{\partial x} \mid_{x=1} = 0,$$

$$D_i \frac{\partial C_i}{\partial r} \mid_{r=0} = \sum_{j=1}^{M_2} v_j^i W_j, if x = I_{ap}/2,$$

$$D_i \frac{\partial C_i}{\partial r} \mid_{r=0} = 0, if x \neq I_{ap}/2,$$

$$D_i \frac{\partial C_i}{\partial r} \mid_{r=D_{ap}/2} = 0,$$

where $i = 1, 2, ..., n; I_{ap}, D_{ap}$- device length and diameter, $m; \tilde{N}_i^L$ - gas constituent original concentration at the reactor inlet, mole/ $m^3; v_i^j$ gas phase i-component stoichiometric coefficient in the j-surface reaction; W_j- j-surface reaction velocity mole/(m^3, s) (1) - modified equation system for the gas constituent concentrations with the optional term, allowing for the interim radicals concentrations impact; $\alpha_0; \alpha_{n+1} = 0$; (2) - initial conditions. In this Article we

prove the solvability of the model (1) - (7), solubility and the iterative method stability in solving the system differential equations (1) [**?**].

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