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Mathematical Modelling of the Impact of IR Laser Radiation on an Oncoming Flow of Nanoparticles with Methane

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Abstract

Introduction. The study is devoted to the numerical investigation of laser radiation's effect on an oncoming two-phase flow of nanoparticles and multicomponent hydrocarbon gases. Under such exposure, the hydrogen content in the products increases, and methane is bound into more complex hydrocarbons on the surface of catalytic nanoparticles and in the gas phase. The hot walls of the tube serve as the primary source of heat for the reactive two-phase medium containing catalytic nanoparticles.

Materials and Methods. The main method used is mathematical modelling, which includes the numerical solution of a system of equations for a viscous gas-dust two-phase medium, taking into account chemical reactions and laser radiation. The model accounts for the two-phase gas-dust medium's multicomponent and multi-temperature nature, ordinary differential equations (ODEs) for the temperature of catalytic nanoparticles, ODEs of chemical kinetics, endothermic effects of radical chain reactions, diffusion of light methyl radicals CH_3 and hydrogen atoms H, which initiate methane conversion, as well as absorption of laser radiation by ethylene and particles.

Results. The distributions of parameters characterizing laminar subsonic flows of the gas-dust medium in an axisymmetric tube with chemical reactions have been obtained. It is shown that the absorption of laser radiation by ethylene in the oncoming flow leads to a sharp increase in methane conversion and a predominance of aromatic compounds in the product output.

Discussion and Conclusion. Numerical modelling of the dynamics of reactive two-phase media is of interest for the development of theoretical foundations for the processing of methane into valuable products. The results obtained confirm the need for joint use of mathematical modelling and laboratory experiments in the development of new resource-saving and economically viable technologies for natural gas processing.

Keywords: mathematical modelling, subsonic flows, two-phase medium, laser radiation, chemical reactions

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Оригинальное теоретическое исследование

Математическое моделирование воздействия ИК-лазерного излучения на встречный поток наночастиц с метаном

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Аннотация

Введение. Работа посвящена численному исследованию воздействия лазерного излучения на встречный двухфазный поток наночастиц с многокомпонентным газом из углеводородов. При таком воздействии увеличивается содержание водорода в продуктах и происходит связывание метана в углеводороды более сложного строения на поверхности каталитических наночастиц и в газовой фазе. Горячие стенки трубы являются источником основного прогрева реакционной двухфазной среды с каталитическими наночастицами.

Материалы и методы. В качестве основного метода используется математическое моделирование, включающее численное решение системы уравнений вязкой газопылевой двухфазной среды с учетом химических реакций и лазерного излучения. Модель позволяет одновременно учитывать двухфазную газопылевую среду, многокомпонентность и многотемпературность среды, обыкновенные дифференциальные уравнения (ОДУ) для температуры каталитических наночастиц, ОДУ химической кинетики, эндотермические эффекты радикально-цепных реакций, диффузию легких метильных радикалов CH_3 и атомов водорода H, которые инициируют конверсию метана, поглощение лазерного излучения этиленом и частицами.

Результаты исследования. Получены распределения параметров, характеризующих ламинарные дозвуковые течения газопылевой среды в осесимметричной трубе с химическими реакциями. Показано, что поглощение лазерного излучения этиленом во встречном потоке приводит к резкому увеличению конверсии метана и преимущественному выходу ароматических соединений.

Обсуждение и заключение. Численное моделирование динамики реакционных двухфазных сред представляет интерес для разработки теоретических основ переработки метана в ценные продукты. Полученные результаты естественным образом подтверждают вывод о необходимости совместного использования средств математического моделирования и лабораторных экспериментов для разработки новых ресурсосберегающих и экономически обоснованных технологий переработки природного газа.

Ключевые слова: математическое моделирование, дозвуковые потоки, двухфазная среда, лазерное излучение, химические реакции

Финансирование. Работа выполнена при финансовой поддержке Министерства науки и высшего образования РФ в рамках государственного задания Института катализа СО РАН (проект FWUR–2024–0033).

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Introduction. In laser thermochemistry, the impact of laser radiation on an oncoming two-phase flow of methane and catalytic nanoparticles is considered [1, 2]. In such a flow, at temperatures above 1000 K, methane is converted into ethylene, acetylene, hydrogen, and aromatic compounds [3, 4]. The chemical reactions involved in the conversion of hydrocarbons in the gas phase and on the surface of catalytic nanoparticles are chain reactions involving radicals, which require a description that includes a large number of components and stages, including the convective and diffusive dynamics of active radicals [5]. These chemical reactions generally define an endothermic process, which shifts toward higher product yields with additional energy absorption. Such absorption can be provided by infrared (IR) radiation from a CO_2 laser directed along the flow into the initial zone of chemical transformations [2]. At the same time, the case when laser radiation is directed at the oncoming flow into the region of high methane conversion is of particular interest. The consideration of this case is the purpose of this publication.

The complexity of multicomponent chemical processes, along with heat and mass transfer, requires mathematical modelling of subsonic flows of reactive two-phase media, consisting of gas and solid ultrafine particles. The authors have developed their own CFD code for calculating the dynamics of such media [2]. This code comprehensively considers subsonic multicomponent gas dynamics with volume changes due to chemical reactions, multicomponent dust dynamics, heterogeneous-homogeneous kinetics of radical chain reactions for hydrocarbons, radiation transfer, and absorption. As a simplification of the model, the flow is considered in an axisymmetric cylindrical 2D space.

Materials and Methods

Mathematical Model. IR laser radiation excites vibrational degrees of freedom in ethylene molecules, which appear as products of gas-phase chemical reactions and on the surface of catalytically active nanoparticles. Thermal relaxation of ethylene, which absorbed laser radiation, leads to heating of all components of the gas. The heat exchange between the gas and nanoparticles, occurring in the free molecular regime (for nanoparticles with diameters in the tens of nanometers), tends to bring the temperatures of the particles and gas to thermal equilibrium. The heated walls of the tube provide the bulk of the energy necessary for the highly endothermic conversion of methane.

To study the effect of laser radiation on the oncoming flow of methane and nanoparticles, a mathematical model was developed based on a system of equations for a viscous gas-dust two-phase medium, taking into account chemical reactions and laser radiation [1, 2]. This system of equations is based on the Navier-Stokes equations, using the approximation of small Mach numbers [6, 7]. The system describes significantly subsonic flows (M << 1) with volume changes, small pressure variations, and simultaneous significant increases in velocity due to chemical reactions, laser radiation, heat exchange between the gas and particles, and dissipative processes.

The mathematical model consists of a system of time-parabolic and space-elliptic equations, owing to the solution of the equation for the dynamic pressure component. The model accounts for: a two-phase gas-dust medium; multicomponent and multi-temperature aspects; ODEs for the temperature of catalytic nanoparticles; ODEs for chemical kinetics; endothermic effects of radical chain reactions; diffusion of light methyl radicals (CH_3) and hydrogen atoms (H), which initiate methane conversion; and the absorption of laser radiation by ethylene and particles.

The mass transfer equation for the gas mixture components is given as:

$$\frac{\partial \rho_g Y_m}{\partial t} + \nabla \cdot \left(\rho_g Y_m \vec{v}\right) = -\nabla \cdot \vec{J_m} + R_m, \quad m = \overline{1, M}. \tag{1}$$

The equations for the mass transfer of nanoparticles are:

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot \left(\rho_i \vec{v}\right) = 0, \quad i = \overline{1, N}. \tag{2}$$

The momentum transfer equation is:

$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot \left(\rho \vec{v}\vec{v}\right) + \nabla \pi = \nabla \cdot \overline{\overline{\tau}}. \tag{3}$$

The equations for gas and particle enthalpy are:

$$\frac{\partial}{\partial t}\left(\rho_g h_g + \sum\nolimits_i \rho_i h_i\right) + \nabla \cdot \left(\left(\rho_g h_g + \sum\nolimits_i \rho_i h_i\right)\vec{v}\right) = -\nabla \cdot \vec{q} - \sum\nolimits_i 4\pi s_i^2 n_i \sigma \left(T_i^4 - T_g^4\right) \tag{4}$$

$$+\left(n_g \alpha + \sum\nolimits_{i=1}^{N} n_i \alpha_i\right) F.$$

Condition for the divergence of the velocity vector is:

$$S \equiv \nabla \cdot \vec{v} = \frac{1}{\rho_g C_p T_g}\left(-\sum\nolimits_{i=1}^{N} \rho_i \frac{C_p\left(T_g - T_i\right)}{\zeta_i}\right) + \frac{1}{\rho_g C_p T_g}\left(\nabla \cdot \lambda \nabla T_g + \sum\nolimits_m \rho_g D_{m,mix} \nabla Y_m \nabla h_m\right) \tag{5}$$

$$+\frac{1}{\rho_g}\sum\nolimits_m \frac{M_w}{M_{wm}}\left(\nabla \cdot \rho_g D_{m,mix} \nabla Y_m\right).$$

Equation for the intensity of radiation is:

$$\frac{dF}{dl} + \left(n_g \alpha + \sum\nolimits_{i=1}^{N} n_i \alpha_i\right) F = 0. \tag{6}$$

Equations for the temperature of nanoparticles are:

$$\frac{dT_i}{dt} = \frac{1}{m_i C_{DV}}\left(\alpha_i F - 4\pi s_i^2 \sigma \left(T_i^4 - T_g^4\right) - a\pi \frac{s_i^2}{2} p_g c_t \frac{\gamma + 1}{\gamma - 1}\left(\frac{T_i}{T_g} - 1\right) - Q \cdot R\right). \tag{7}$$

Equations of chemical kinetics are:

$$\frac{\partial \rho_g Y_m}{\partial t} = R_m, \quad m = \overline{1, M}. \tag{8}$$

Here ρ_g is the density of the gas mixture; Y_m is the mass fraction of the m-th gas component; M is the number of components in the gas mixture; $\overrightarrow{J_m}$ is the diffusion flux vector; R_m is the rate of formation or consumption of the m-th component of the mixture; $\vec{v}$ is the velocity of the gas and particle flow; ρ_i is the density of the i-th particle; N is the number of particle fractions; $\rho = \rho_g + \sum_{i=1}^{N} \rho_i$ is the total density of the gas and particles; $\pi = \rho_g - \rho_0$ is the dynamic pressure component; where ρ_g is the pressure and ρ_0 is the constant pressure in the region; $\overline{\overline{\tau}}$ is the viscous stress tensor; h_g is the enthalpy of the gas, h_i is the enthalpy of each particle fraction, $\vec{q}$ is the heat flux vector, n_g is the average concentration of absorbing gas molecules per unit volume; n_i is the concentration of particles in the dust fraction; F is the radiation intensity; α, α_i are the absorption coefficients; T_g is the gas temperature; T_i is the temperature of the particles in the dust fraction; s_i is the particle radius; σ is the Stefan-Boltzmann constant; C_p is the heat capacity of the mixture at constant pressure; $\zeta_i = \dfrac{2m_i C_{DV}(\gamma-1)T_g}{a\pi s_i^2 p_g c_t(\gamma+1)}$ is the thermal relaxation time of the particle in the medium; m_i is the mass of the particle; C_{DV} is the heat capacity of the particle material at constant volume; γ is the adiabatic index of the gas mixture; a is the accommodation coefficient; c_t is the average thermal velocity of gas molecules; M_w is the average molecular weight of the mixture; M_{wm} is the molecular weight of the m-th component of the mixture; l is the laser radiation propagation coordinate; c_t is the average thermal velocity of gas molecules; Q is the heat effect of the reaction; R is the number of transformations per unit time.

Information on the expressions for determining the diffusion flux vector, the rate of formation or consumption of gas components, the viscous stress tensor, the enthalpy of each particle fraction, the heat flux vector, absorption coefficients, thermal relaxation time, the average thermal velocity of gas molecules, and the heat effect of the reaction is provided in [1].

Chemical processes in the heated medium are calculated based on a kinetic scheme of interconnected heterogeneous and homogeneous radical-chain reactions, which includes 40 elementary stages and 15 components of the gas mixture. The scheme was designed for a temperature range from 900 K to 1400 K [8]. The laser beam diameter, power, and duration are parameters that are defined in the initial and boundary conditions. Further, the use of continuous CO_2 laser radiation is assumed, although single-pulse and pulse-periodic radiation modes for the CO_2 laser may also be studied.

The presented system of equations is complemented by initial and boundary conditions. The initial conditions include the concentrations of gas components Y_m^0, particle concentrations n_i^0, gas temperature T_g^0, particle temperature T_i^0, pressure p^0, and flow velocity $\overrightarrow{v^0}$. The boundary conditions consider the inflow conditions $(Y_m^{in}, n_i^{in}, T_g^{in}, T_i^{in}, p^{in}, \overrightarrow{v^{in}})$, outflow conditions p^{out}, and adhesion conditions $(T_g^{bound}, \vec{v} = 0)$.

During one time integration step, the equations of chemical kinetics (8) are solved sequentially to account for the contribution of chemical reactions to the component composition, the equations for particle temperature (7) and laser radiation (6) are solved, and the system of equations (1)–(4) is integrated without considering the dynamic pressure component. The values of the gas component and nanoparticle densities, the total enthalpy of the gas and particles, and the preliminary velocity vector are obtained. From the computed values, the gas mixture temperature, gas component concentrations, and nanoparticle concentrations are derived. At the final stage, Poisson's equation is solved using the condition for the divergence of the velocity vector (5) to find the dynamic pressure component π\piπ, and the velocity vector is corrected.

The described computational algorithm was implemented in C++ using MPI parallel computing technology. The most labor-intensive step is the calculation of the chemical kinetics equations [9], as it involves solving a stiff system of equations that includes dozens of gas mixture components. Another labor-intensive step is solving Poisson's equation for the dynamic pressure component, where it is necessary to solve a system of linear algebraic equations (SLAE), the size of which depends on the computational grid. The computational algorithm for individual equations was tested on known solutions. The algorithm was previously tested in limiting cases on analytical solutions for model problems of Poiseuille flow, Couette flow, and heat conduction with a chemical reaction (in the flat variant), as well as experimental data on ethane pyrolysis. The convergence of the numerical method was verified and confirmed on a sequence of refined grids.

Results

Inlet and Outlet Flows in the Computational Domain. The cylindrical shape of the computational domain is determined by the typical design of reactors in chemical technologies and the well-studied nature of flows in straight pipes with circular cross-sections. The cross-section of the laser radiation beam, in the geometric optics approximation, is often also circular, with the radius adjustable by optical elements. The coaxial propagation of the laser beam through a circular tube is easily achievable in laboratory experiments. For computational experiments aimed at determining the influence of laser radiation on the counterflow of reagents, such a configuration of the computational domain, along with the radiation, is of particular interest. This setup eliminates the need to calculate flow distributions over the azimuthal angle in the cylindrical coordinate system, reducing the problem to a two-dimensional formulation, which greatly simplifies the development of the computational algorithm. The main expected result of introducing laser radiation into the reaction medium is the creation of a high-temperature region, which serves as a source of additional radicals outside this region. This significantly enhances the reactive capacity of the system at the outlet and allows for higher methane conversion rates under otherwise equal conditions.

The computational domain (Fig. 1) represents a cylindrical tube with a total length of 600 mm and a diameter of 20 mm. The domain consists of four zones from **A** to **D**. Zone **A** has reduced wall temperatures and is intended for the calculation of radiation input. It is isolated from the main reaction zone **C** by an annular inlet **1** for relatively cold methane. In zone **B**, the walls heat the methane to a certain temperature. Reaction zone **C** is 330 mm long and is bounded by an annular inlet **3** for the gas-dust mixture and an annular outlet **2** for the reaction products. In zone **D**, a flow of methane with nanoparticles is formed, moving towards the laser radiation. Such an arrangement of the reaction zone is necessary to organize the impact of laser radiation on the reacting mixture in the product outlet area and to prevent overheating of the tube's end walls.

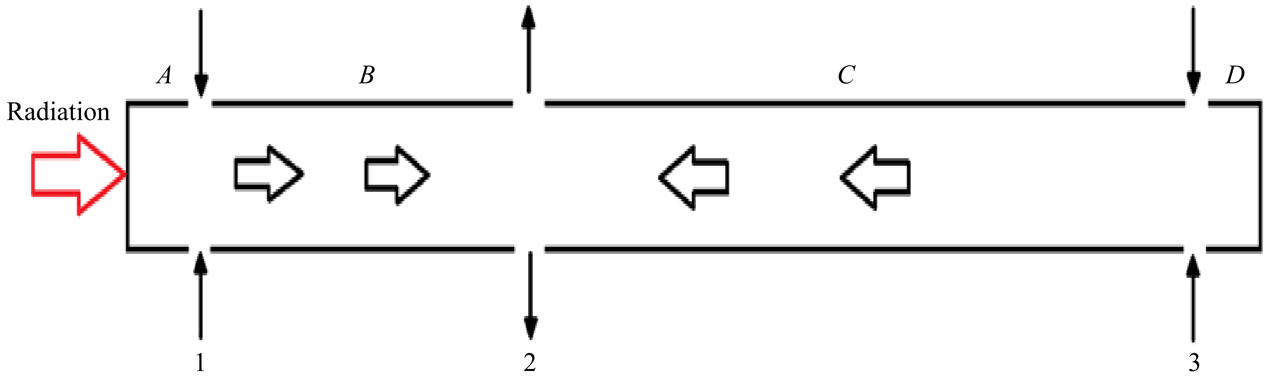

Fig. 1. Scheme of the calculation area with inlet and outlet flows

Initial and boundary conditions. At the initial moment, the area is filled with methane at a temperature of 973 K and a pressure of 101.325 Pa. Inlets **1** and **3** define conditions for the inflow of a flow with a specified constant flow rate of 10 L/h (10 % from inlet 1, 90 % from inlet 3) and the composition of the mixture. A gas-particle mixture (methane and catalytic nanoparticles with a radius of $5 \cdot 10^{-9}$ m, and a concentration of $1.2 \cdot 10^{18}$ m^{-3}) is supplied through inlet **3**, preheated to 1173 K. Energy is introduced into the reaction zone through walls **B** and **C**, which are at a temperature of 1173 K. As it moves through the reaction zone, the gas and particles are heated from the walls to the center. A relatively cold methane with a temperature of 573 K is supplied through inlet **1**. At the wall temperature of 1173 K, it remains inert and flows counter to the gas-particle mixture. The mixing of flows and the output of reaction products occur at outlet **2**. The wall temperature in zones **A** and **D** is 573 K. To the left along the axis, radiation from a 30 W CO_2 laser with a beam diameter of 12 mm is introduced. The width of the annular inlets 1 and 3 is 5 mm, and the outlet 2 is 8 mm.

The described problem is solved in a cylindrical coordinate system for the case of axisymmetric flow. The calculations are based on a 2D grid of rectangles, with 6000 cells, a spatial step of $h=10^{-3}$, and a time step of $\Delta t = 10^{-5}$.

For the chosen size and initial concentration of nanoparticles, particle aggregation into fractal agglomerates may occur, but the time for this process significantly exceeds the residence time of the nanoparticles in zone **C**. Furthermore, the total surface area of fractal agglomerates changes little, maintaining a total catalytic surface sufficient for methane conversion. For the given parameters, the ratio of the thermal conductivity length of the gas to the radius of the pipe and the ratio of the diffusion length of a hydrogen atom to the radius is greater than 1. This defines the heating of the medium in the pipe. The filling of the entire mixture with hydrogen atoms radially ensures the occurrence of radical chain reactions with methane and secondary hydrocarbons. The mixing of the relatively cold counterflow of methane in the annular output zone 2 and the absorption of laser radiation provides the cooling of the gas-particle mixture at the outlet.

Flow without Laser Radiation Input. Let's consider the flow of a two-phase gas-particle mixture with chemical reactions in the axisymmetric pipe presented in Fig. 1, without the introduction of laser radiation. The conversion of methane is an endothermic process, and the energy required to initiate the reactions is supplied to the system through the continuous heating of the walls of the area.

Counterflows of the supplied gas-particle mixture through the annular inlet **3** on the side surface of the pipe mix effectively, reverse, and form a laminar flow along the axis (from right to left). At a distance of one diameter of the pipe from inlet **3**, under the influence of wall heating, the velocity reaches its maximum value of 11 cm/s (Fig. 2). In this area, the conversion of methane begins, accompanied by a redistribution of reaction products. The presence of hydrogen in the products leads to a significant change in the volume of the medium, causing flow deceleration that starts at a distance of two diameters from inlet **3**. The decrease in velocity corresponds to an increase in particle concentration in the second part of the reaction zone (closer to outlet 2). The presence of inlet **1** also affects the formation of gas flows, resulting in the methane supplied to this area limiting the reaction zone. The gas-particle flow and the methane flow mix, creating a deceleration zone at the outlet **2** (Fig. 2).

The maximum concentration of particles, which is twice that of the concentration at inlet **3**, is observed at outlet **2** (Fig. 3). The temperature of the mixture in the reaction zone is close to the wall temperature (Fig. 4), illustrating the condition in which the energy supplied from the walls of the pipe is sufficient to heat the entire area and facilitate the endothermic chemical reactions. The special design of the pipe also plays a role here — lower temperatures at the end walls due to gas insulation in these areas protect the windows (for potential laser radiation input) from heating.

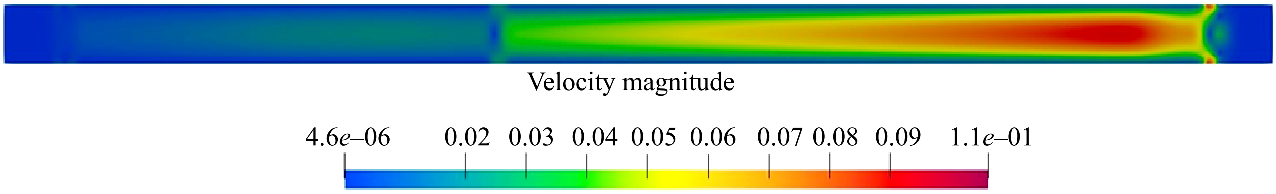

Fig. 2. Velocity distribution, m/s

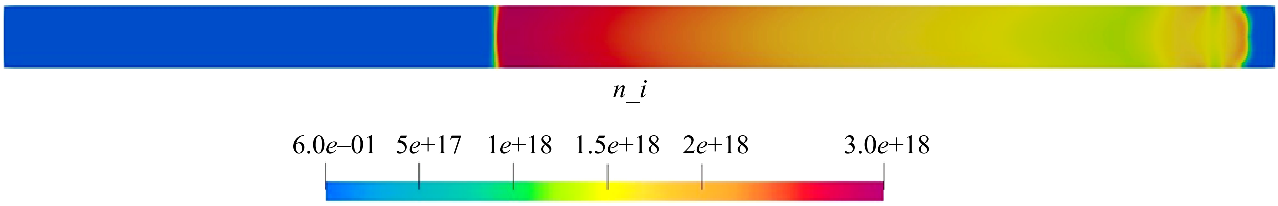

Fig. 3. Nanoparticle distribution, m^{-3}

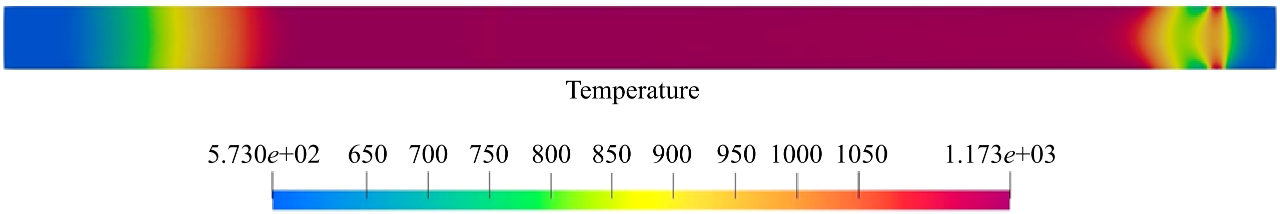

Fig. 4. Temperature distribution, K

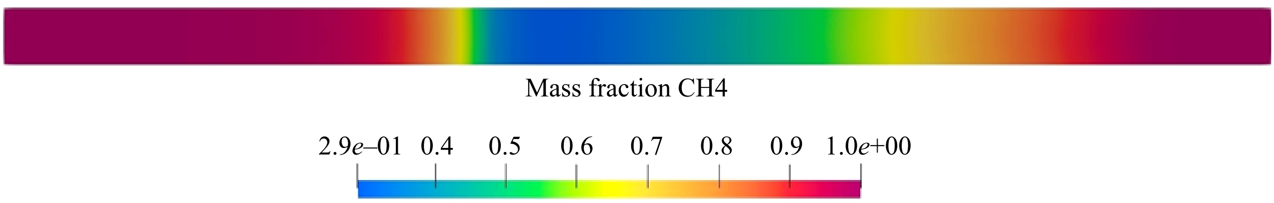

Fig. 5. Methane mass fraction distribution

Chemical reactions are initiated at a distance of one pipe diameter from inlet **3** due to wall heating and proceed throughout most of the reaction zone **C**, with more active methane conversion (71 %) near outlet **2**. The maximum methane conversion is observed in this area due to the accumulation of nanoparticles (Figs. 3, 5), which act as active centers for chemical reactions, and the mixture's temperature, which is approximately equal to the wall temperature. As the gas-particle flow moves, reaction products are formed and accumulate, with their maximum concentrations occurring near outlet **2**. The main products are aromatic compounds — 31.5 %, ethylene — 16.2 %, and hydrogen — 10.0 %. At outlet **2**, the methane conversion is 65.0 %, as the reaction mixture mixes with the counterflow of methane (10.0 % comes from inlet 1, 90 % from inlet **3**).

Effect of Laser Radiation. Let's consider the results of the calculation for a chemically active two-phase flow in the presence of laser radiation. A laser beam with a power of 30 W and a diameter of 12 mm is introduced along the axis of the pipe through the left end.

The laser radiation, entering the pipe from the left, passes through the buffer zone filled with optically transparent methane and is absorbed in the outflow area by nanoparticles and ethylene (Fig. 6).

The energy input leads to the formation of a high-temperature region, with values reaching 1364 K (Fig. 7). The shift of the elevated temperature into the buffer zone is explained by the diffusion of ethylene and hydrogen, which absorb the radiation, with hydrogen having thermal conductivity several times higher than other components of the mixture. Despite the temperature increase in this area by almost 200 K compared to the calculation without radiation, the flow velocity and, consequently, the particle concentration do not change throughout the pipe volume (Figs. 8, 9). The energy from the laser radiation, along with the temperature increase, is consumed by endothermic chemical reactions.

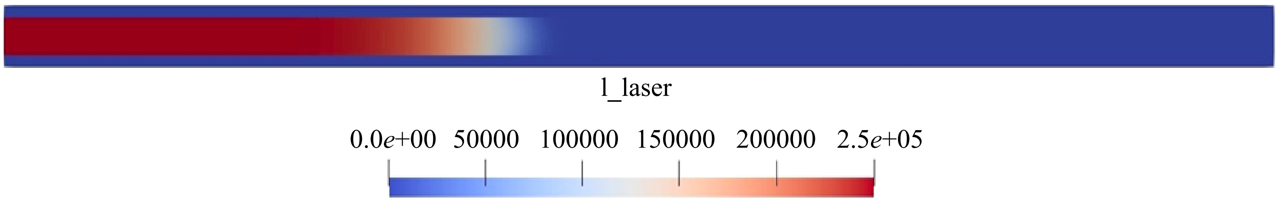

Fig. 6. Radiation intensity distribution, W/m^2

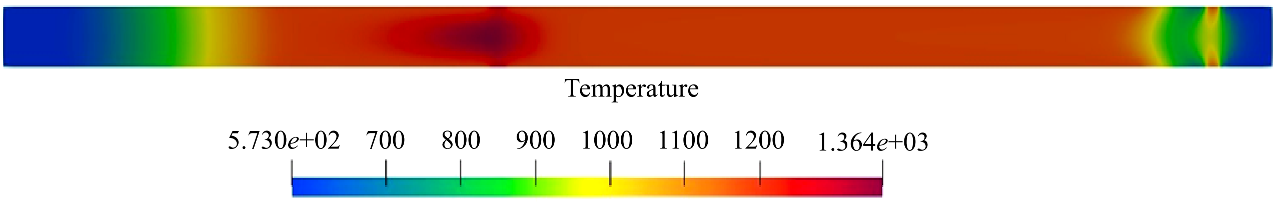

Fig. 7. Temperature distribution, K

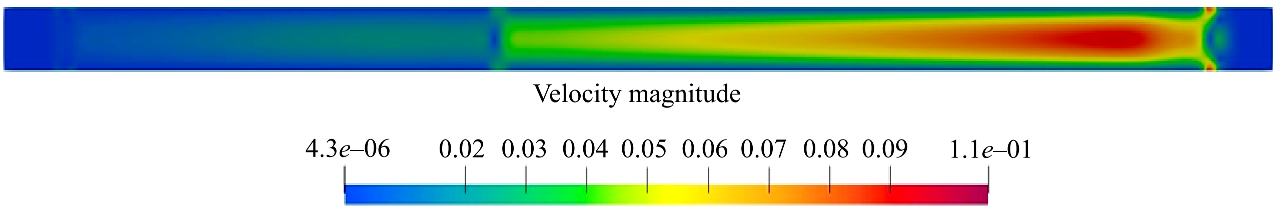

Fig. 8. Velocity distribution, m/s

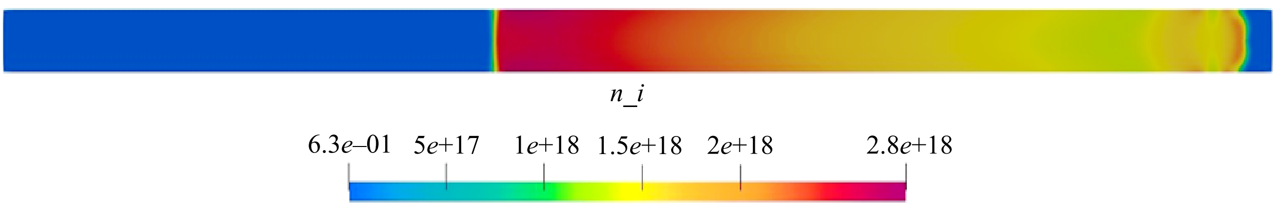

Fig. 9. Nanoparticle distribution, m^{-3}

Figures 10–12 show the distribution of the main components of the gas mixture along the pipe. From the graphs, it is evident, as in the case without radiation, that there is a gradual increase in reaction products toward outlet **2**, with methane conversion reaching 73 %. However, with the introduction of laser radiation, a significant redistribution of the component composition occurs along the pipe. The highest mass fractions of hydrogen (Fig. 11) and aromatic compounds (Fig. 12) are observed near outlet **2**, as these products form at temperatures above 1300 K, provided by the laser radiation input. The mass fraction of ethane in this area rapidly decreases, as it undergoes pyrolysis at such high temperatures. The maximum ethylene fraction of 19 % is observed in the central part of the reactor, decreasing to 6 % toward the outlet. The appearance of about 5 % hydrogen in the left "protected" area of the pipe is explained by its diffusion.

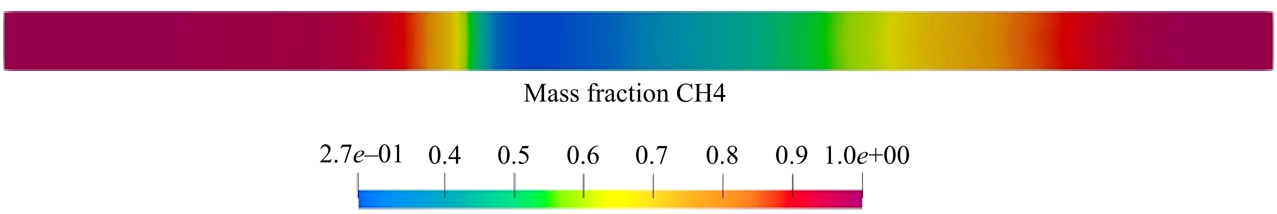

Fig. 10. Methane mass fraction distribution

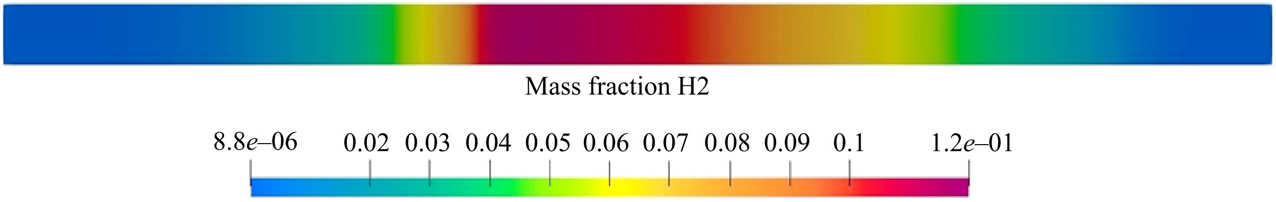

Fig. 11. Hydrogen mass fraction distribution

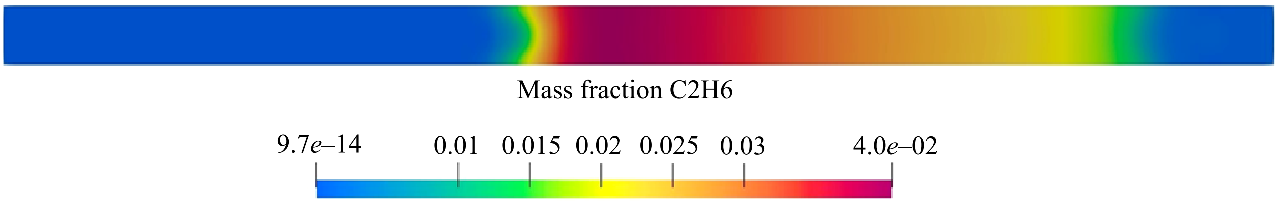

Fig. 12. Aromatic compounds mass fraction distribution

Since the counterflows of methane mix at the pipe outlet, the observed methane conversion decreases to 69.0 %, with the following mass fraction distribution of target reaction products: aromatic compounds — 44.0 %, ethylene — 6.0 %, and hydrogen — 11.6 %.

To study the influence of parameters in the computational experiment, calculations were performed for other values of wall temperatures in reaction zone **C**, ranging from 1073 K to 1173 K, with all other initial and boundary conditions unchanged. In the presence of laser radiation, the dependence of methane conversion on wall temperature is linear: with a 25 K increase in the mixture temperature, the additional methane conversion is around 10 %, primarily forming aromatic compounds. This is due to the fact that, upon reaching a certain temperature, the kinetics of the chemical reactions shift toward the formation of these compounds.

Discussion and Conclusion. Mathematical modelling of chemically active two-phase gas-particle flows was carried out using a self-developed program. The program is designed for calculations in cylindrical coordinates for axisymmetric subsonic flows with small pressure variations. The numerical algorithm imposes no restrictions on changes in flow velocity within the computational domain or on significant volume changes due to chemical reactions. The developed program was adapted to study methane conversion in a pipe with counterflows of reacting gas and IR laser radiation. In a series of computational experiments without radiation and with 30 W radiation, the effect of laser radiation on the dynamics of the chemically active counterflow of the gas-particle mixture was investigated.

It was found that relatively low-power and low-intensity IR laser radiation, around 30 W/cm^2, absorbed directly in the gas, has a strong impact on the counterflow of the two-phase nanoparticle and hydrocarbon gas mixture. This influence results in the creation of a higher temperature zone at the outlet of the reaction medium. Elevated temperatures and the heat power input in the presence of radiation lead to a shift in methane conversion products toward increased yields of aromatic hydrocarbons. The increase in aromatic output is achieved by introducing laser energy at the final stage of the chemical process. The quenching of the resulting products occurs as the reaction mixture exits the laser radiation zone. Numerical modelling of the dynamics of reactive two-phase media is of interest for developing the theoretical foundations for methane conversion into valuable products. The results naturally confirm the conclusion that mathematical modelling, combined with laboratory experiments, is essential for developing new resource-efficient and economically viable technologies for natural gas processing.

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