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SIMULATION OF NONEQUILIBRIUM HYDROCARBON GAS FLOW IN THE HIGH ASPECT RATIO CHANNELS WITH PHASE TRANSITION AND HIGH HEAT INTENSITY

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I. Abstract

An important task when developing power systems is to enable specified thermal conditions for hydrocarbon flow in the cooling channels with high aspect ratio. High temperature level of hydrocarbon composition and heat transfer intensity result in nonequilibrium flow with phase transition following by soot formation on the inner wall of the channel. The presented work is devoted to one-dimensional and two-dimensional flow simulations of heat exchange problem in the channels with external heat supply consider thermal decomposition of hydrocarbon gas. The one-dimensional mathematical model solves conservation laws equation system for flow and uses global reaction to simulate the macrokinetic processes of hydrocarbon decomposition. The two-dimensional high-level mathematical model also solves conservation laws equation system for flow, but for hydrocarbon thermal decomposition it uses reduced kinetic mechanism. The paper will present some numerical results obtained for a hydrocarbon flow in the channel under different heat loads, based on which one- and two-dimensional mathematical models were verified. The parametric research of flow conditions depending on channel shape, mass loading and heat load was held.

II. Introduction

The main issue of modern propulsion plants is the cooling of the flow duct due to high levels of heat load, since even composite materials can't withstand it. This requirement leads to the idea of using hydrocarbon endothermic compositions, because of their capability to decompose into lighter species providing additional heat sink [1].

The one-dimensional and multidimensional simulations are the powerful tools which allow to determine the possible characteristics for the cooling systems of the propulsion plants on gaseous hydrocarbon compositions. Thus, the development of a mathematical model for flow patterns determination of gaseous hydrocarbon compositions under high heat load is the important task. The necessity to conduct a large number of simulations for parametric research results in requirement of simple and reliable tool with low computational cost.

This paper presents some numerical results obtained for gaseous *n*-pentane (*n*-C_5H_{12}) flow in a channel with high aspect ratio under different heat loads and flow parameters to verify one-dimensional model on the basis of the two-dimensional simulations results.

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III. Two-dimensional mathematical model

The transient, chemically reacting flow within the cooling channel (fig. 1) was simulated with high-level software suite which solves the two-dimensional Favre Averaged Navier-Stokes equations with reduced kinetic mechanism. Eddy Dissipation Concept (EDC) [2] model was used to include detailed chemical mechanisms in turbulent flow. Turbulence effects were simulated with k-ω SST turbulence closure model. A mass flux boundary condition was used on the inflow cross-section, and a pressure boundary condition - on the outflow. The solid wall was imposed with heat flux, no-slip conditions.

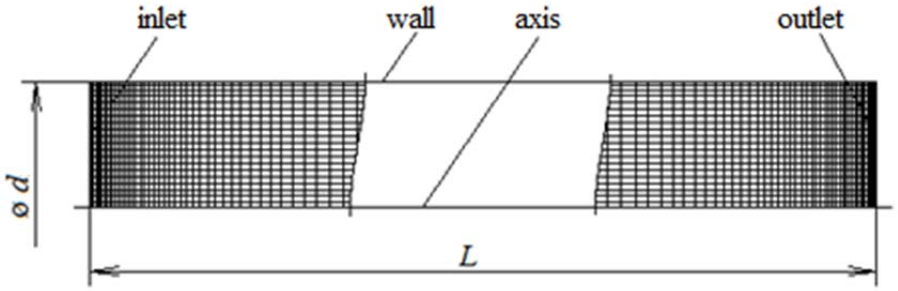

Fig. 1. Geometry and grid layout for the two-dimensional simulation

The modeling of hydrocarbon decomposition is the pivotal part of presented mathematical modeling. Detailed chemical kinetic descriptions of hydrocarbon thermal decomposition may require the tracking of hundreds of chemical species and thousands of reactions. The modern CPU time and computer memory limitations prohibit implementation of fully detailed description of thermal decomposition into multi-dimensional CFD (computational fluid dynamics) simulations. Therefore, it is important to minimize the number of species and reactions while retaining main features of the detailed chemistry [3].

In this paper the decomposition of gaseous n-C_5H_{12} was modeled with reduced kinetic mechanism of 19 species and 36 forward and backward reactions. The approach used here was to reduce mechanism of n-pentane thermal decomposition by elimination insignificant species and reactions under considered conditions ($p < 2$ MPa, $T < 1000$ K).

These two-dimensional simulations require considerable computational resources compared to one-dimensional calculations and thus it is not very convenient to use them for parametric research. However, the two-dimensional simulation are more detailed and less dependent on empirical data, they include more of the detailed chemistry of hydrocarbon decomposition process.

In fig. 2 the flow parameters distributions are presented which were obtained as a result of a two-dimensional simulation of n-C_5H_{12} decomposition under heat flux $q = 1{,}0$ MW/m^2.

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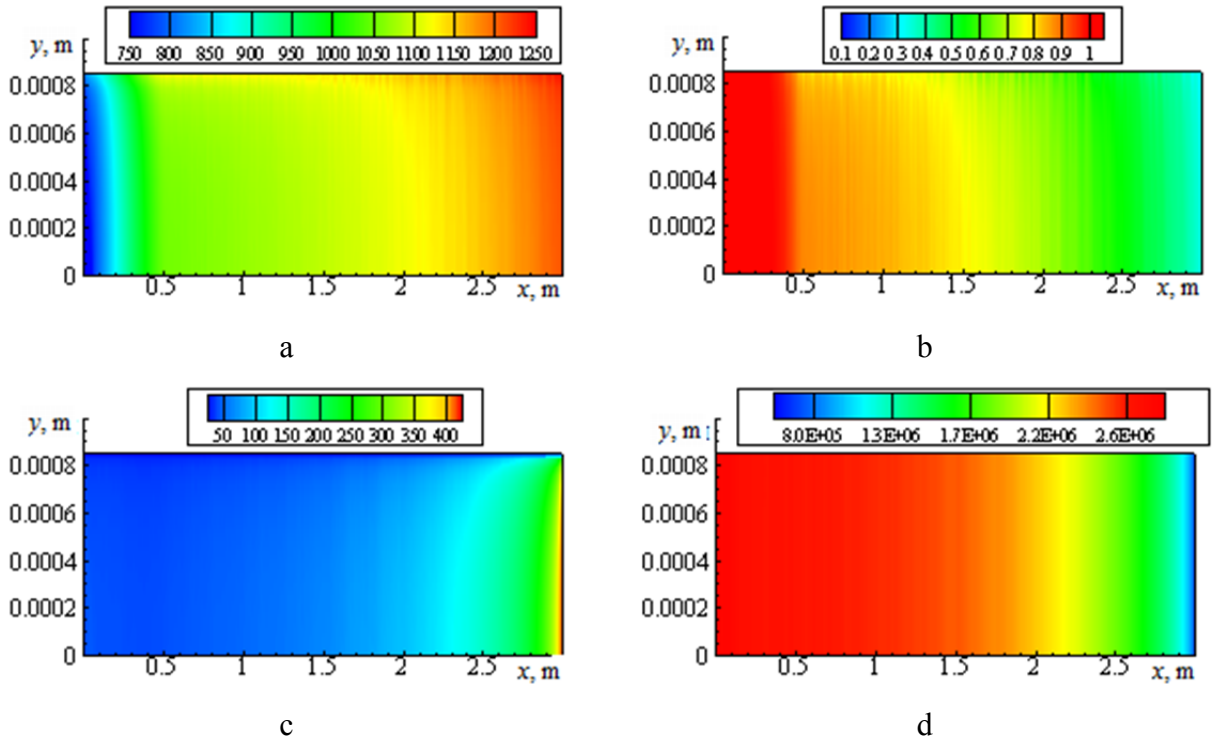

Fig. 2. Distribution of *n*-C_5H_{12} flow parameters in round channel under heat flux 1,0 MW/m^2:

a – temperature; b – *n*-C_5H_{12} mass fraction; c – axial velocity, d – static pressure

The main rationale of these numerical simulations was to verify the one-dimensional mathematical model as a tool needed to design a cooling system of a propulsion plants. In particular, for cooling channels with high aspect ratio, the goal of this effort was to predict critical quantities and flow patterns.

IV. One-dimensional mathematical model

A one-dimensional mathematical model was developed to analyze hydrocarbon flow and thermal decomposition in the channel with high aspect ratio in a quick and inexpensive manner. The steady state flow of gaseous *n*-C_5H_{12} was simulated with one-dimensional model that solves a system of differential equations for the conservation of mass flow, momentum and energy in the following form:

$$\begin{cases} \dfrac{\partial}{\partial x}(\rho W) = 0; \\ \dfrac{\partial}{\partial x}(pF + GW) = \tau\Pi; \\ \dfrac{\partial}{\partial x}(h_\Sigma) = \dfrac{\Pi q}{G} \end{cases}$$

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with x – channel axial coordinate; W – flow velocity; $\Pi = \pi d_к$ – channel perimeter; $F = \pi d_к^2/4$ - channel cross-section surface; $G = \rho WF$ – mass flow rate; $\tau = C_f \frac{\rho W^2}{2}$ - shear stress; $C_f = \frac{2 \cdot 0{,}332}{\sqrt{Re}}$ - drag coefficient [4]; $Re = Wd_к\rho/\mu$ – Reynolds number; $h_\Sigma = h + W^2/2$ – stagnation enthalpy, h – thermodynamic enthalpy of *n*-pentane; q – heat-flux density.

The system is closed by ideal-gas law:

$$\frac{p}{\rho} = \frac{R_\mu}{M_\Sigma} T.$$

In this law R_μ - universal gas constant, M_Σ – molar mass of gaseous mixture, that depends on mass fraction of initial reactant and its product and can be estimated as:

$$M_\Sigma = \frac{1}{\frac{g}{M_{init}} + \frac{1-g}{M_{pr}}},$$

with M_{init}, M_{pr} – molar mass of initial reactant and its product accordingly; g – mass fraction of initial reactant.

The thermal decomposition of gaseous hydrocarbon was modeled with a quasi-global reaction, in which the initial reactant decomposed to the final products. The thermophysical properties of a n-pentane and its decomposition products in each cross-section of the channel can be determined depending on the local temperature and the mass fraction of the initial reactant. For this, the known thermophysical properties of the initial reactant and the equilibrium products of its decomposition are used, depending on the temperature:

$$\begin{aligned}
h(g,T) &= h^{pr}(T)\cdot(1-g) + g\cdot h^{init}(T),\\
C_p(g,T) &= C_p^{pr}(T)\cdot(1-g) + g\cdot C_p^{init}(T),\\
\mu(g,T) &= \mu^{pr}(T)\cdot(1-g) + g\cdot \mu^{init}(T),\\
\lambda(g,T) &= \lambda^{pr}(T)\cdot(1-g) + g\cdot \lambda^{init}(T).
\end{aligned}$$

In the abovementioned equations h, h^{pr}, h^{init} – thermodynamic enthalpy of mixture, equilibrium decomposition products and initial reactant accordingly; C_p, C_p^{pr}, C_p^{init} – specific heat of mixture, equilibrium decomposition products and initial reactant; μ, μ^{pr}, μ^{init} - coefficient of dynamic viscosity of mixture, equilibrium decomposition products and initial reactant; λ, λ^{pr}, λ^{init} – heat conductivity of mixture, equilibrium decomposition products and initial reactant.

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The dependence of the thermophysical properties of the initial reactant and the equilibrium products of its decomposition on temperature were determined with the thermodynamic calculations carried out using the software TERRA.

The completeness of decomposition reaction was expressed in terms of mass fraction of the initial reactant:

$$g = \frac{CM_{init}}{\rho} = \frac{CM_{init} R_\mu T}{pM_\Sigma}$$

with C – molar concentration of initial reactants. исходного вещества.

The speed of the global decomposition reaction under constant volume condition was determined as the derivative of the molar concentration of the initial reactant with respect to time. After replacing the time derivative by the axial length derivative, the expression for molar concentration has taken the following form:

$$-\frac{dC}{dx} = \frac{kC}{W},$$

with $k = k_0 \exp\left(-\frac{E_a}{R_\mu T}\right)$ – reaction rate constant; E_a – activation energy, k_0 – pre-exponential factor.

The solution of the considered system of equations was performed using the discretization of parameters along the channel axis with subsequent integration by an explicit method.

V. Verification and results

Verification of mathematical models is carried out by comparing the results of calculations obtained with a high-level two-dimensional mathematical model and a one-dimensional model. The collation between the one-dimensional and two-dimensional calculations are presented below. The simulations were made for the channel with diameter $d = 1{,}7 \cdot 10^{-3}$ m, heat flux $q = 0{,}5 \ldots 1{,}5$ MW/m^2 with initial temperature of gaseous n-C_5H_{12} $T_0 = 750$ K. The temperature and pressure distribution along the channel axis obtained by the one-dimensional and the two-dimensional simulations are presented on fig. 3. The figures show reasonable agreement between the two dimensional and one-dimensional results everywhere except high heat fluxes. These results indicate that the present one-dimensional model can simulate reasonably well the flow and heat-transfer in the channels with high aspect ratio with minimal computational cost.

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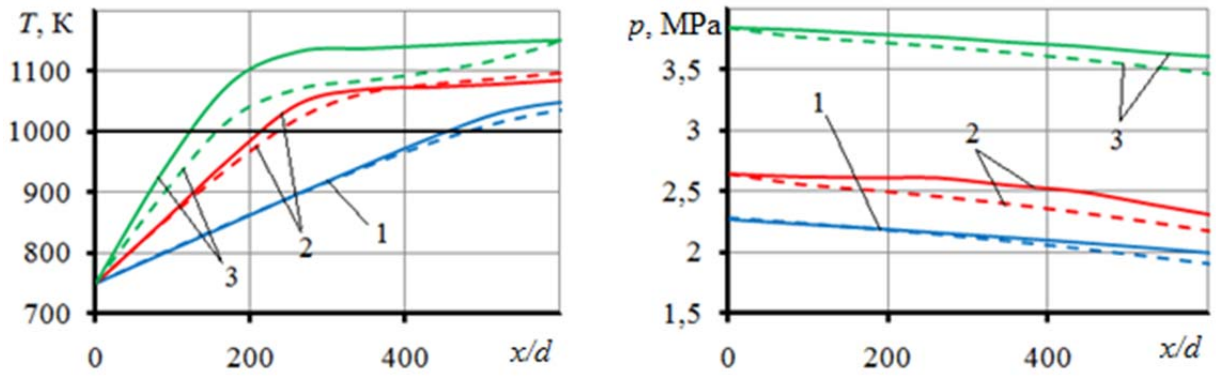

(a) (b)

Fig. 3. Temperature (a) and pressure (b) distribution along the channel relative length *x/d*: solid line – two-dimensional simulation, broken line – one-dimensional simulation. 1 – *q* = 0,5 MW/m^2, 2 – *q* = 1,0 MW/m^2, 3 – *q* = 1,5 MW/m^2

The limit length of channel L_{lim} was considered as a criterion of gaseous n-C_5H_{12} efficiency for heat loaded walls cooling. This is the length at which the temperature of hydrocarbon comes up to 1000 K, and soot formation process is activated. The generalization of computational results obtained by verified one-dimensional model allowed to expose interaction between L_{lim}, Re, and q (fig. 4).

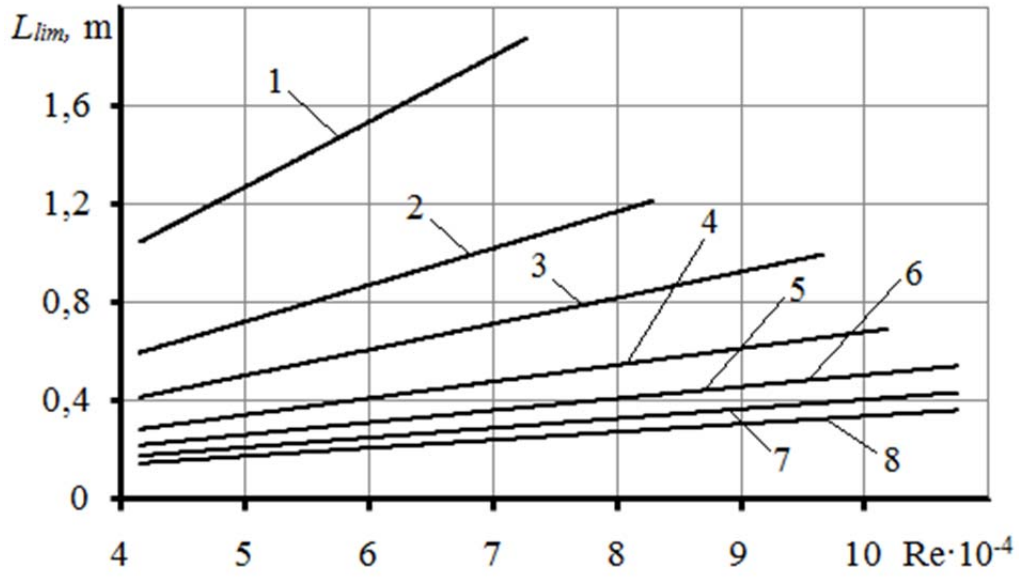

Fig. 4. The dependence of the limit length on Re with various *q*, MW/m^2: 1 – 0,2 , 2 - 0,35, 3 - 0,5, 4 – 0,75, 5 - 1,0, 6 - 1,25, 7 – 1,5

The figures shows that with Re increase while fixed heat flux the limit length of channel increases.

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VI. Summary

Numerical simulations of varying levels of fidelity were carried out to verify the one-dimensional mathematical model of thermal decomposition of gaseous hydrocarbon in the channels with high aspect ratio under different heat flux values. The results obtained by the two-dimensional and one-dimensional simulation showed reasonable agreement with the error not exceeding 7%. Therefore, the one-dimensional model may be successfully used for parametric research of hydrocarbon thermal decomposition. The two-dimensional model may be used for detail analysis of flow structure and chemical transformations in the heat loaded channels with hydrocarbon compositions.

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