NUMERICAL SIMULATION OF THE CONJUGATE HEAT TRANSFER IN THE COOLING SYSTEM OF THE COMBUSTION CHAMBERS OF THE AVIATION RAMJET ON THE ENDOTHERMIC FUELS

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Abstract. *The paper represents 3D mathematical model of conjugated heat exchange in the cooling systems of the aviation ramjet engines. The systems use cooling capacity of the turbulent endothermic fuel flows in heated curvilinear rough channels surrounding the combustion chamber. Simplest one-step model based on substitution of the real hydrocarbon substances by some fictitious medium is used for description of thermal decomposition of the endothermic fuels. The one-step pyrolytic reaction mechanism describes the fictitious medium decomposition without intermediate reactions. In addition to the standard model based on the Navier-Stokes equations, the mathematical model includes a partial differential equation for computation of a local decomposition degree of the fictitious medium in curvilinear channels to avoid computation of residence time. Energy equation has an extra source term describing the endothermic effect of the hydrocarbon substance pyrolysis. The paper represents results of the numerical experiments with pentane under supercritical pressure as the endothermic fuel.*

1   INTRODUCTION

Cooling of an aircraft and a combustion chamber of its engine is the most important problem for flight Mach number higher than 6 [1]. Now the main trend is to use the cooling capacity of the engine fuel for thermal protection of the combustion chamber. Prior to injection and burning, the hydrocarbon fuel flows through the cooling system surrounding the combustion chamber. The fuel consumption is relatively small because the engine thrust must compensate the aerodynamic friction losses on high flight altitudes. As a result, minimum fuel can be used for thermal protection of the combustion chamber, average specific heat flux from the combustion products to the chamber wall is ~ 1 MW/m^2 and higher.

Some natural hydrocarbons (ethane C_2H_6, propane C_3H_8, butane C_4H_{10} and pentane C_5H_{12}) can be decomposed into mixture of simpler hydrocarbons with low molecular weights at high temperature. The thermal decomposition is an endothermic process, i.e. it takes place with heat absorption. Hydrocarbons absorbed heat at the decomposition and used as a fuel for high speed aircrafts are called as "endothermic fuels" (EF) [2, 3]. Attractive property of EF is an opportunity to use an additional cooling effect [4]. This fact results in intensive experimental and numerical studies of heat transfer in EF with endothermic pyrolytic reactions under supercritical pressure.

The simplest model of EF thermal decomposition is the most preferable for the engineering applications. Instead of real EF, the model uses some fictitious substance that decomposes without any intermediate reactions (so-called one-step pyrolytic mechanism) [5, 6]. Empirical constants and functions described the fictitious substance decomposition are chosen for obtaining good agreement between computed and experimental data for real EF [7, 8]. Advantage of the simplest model is the least computational efforts as compared with more complicated models. It should be emphasized that the combustion chamber and its cooling system should be computed in the coupled manner. So numerical simulation of aviation engines require not only accurate mathematical models, but also very efficient solvers for minimizing of the computational work.

Cooling system of the combustion chamber walls is shown in Fig. 1. EF comes to the cooling system and absorbs heat through enthalpy variation. Once the EF temperature exceeds a threshold level, the pyrolytic process can enhance the heat-absorbing capacity through chemical energy changes of EF. Note that reactivity of decomposition products (DP) is higher than reactivity of EF. This fact makes it possible to improve organization of the combustion process in the chamber. After that DP comes to the combustion chamber through pylons.

The aim of this work is: 1) development of 3D mathematical model of turbulent flows of thermal decomposed EF under supercritical pressure in curved rough channels of the cooling system; 2) numerical study of the conjugate heat transfer in panel of the cooling system.
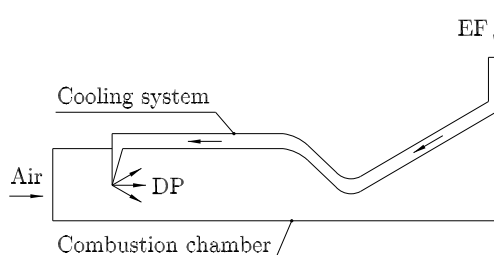

Figure 1: Cooling system of the combustion chamber walls of the aviation ramjet engines.

2 MATHEMATICAL MODEL OF ENDOTHERMIC FUEL DECOMPOSITION

The simplest mathematical model of conjugated heat exchange in the cooling systems is based on the following assumption: EF is replaced by a fictitious medium (FM), thermal properties of FM (density, viscosity, thermal conductivity and heat capacity) depend on the pressure, temperature and function Ψ, hereinafter referred as a local decomposition degree. In addition to the equations of continuity, momentum, turbulence, energy (for FM flow) and thermal conductivity (for channel), the mathematical model should include an equation for the local decomposition degree Ψ. Energy equation should include a source term accounting the endothermic effect of the EF decomposition.

2.1 Computation of the decomposition degree

The decomposition degree is a quantitative measure of the EF conversion into mixture of the simpler hydrocarbon compounds. Assume that a vessel is filled by of EF and N_0 is the number of EF molecules in the initial time τ_0. The equation described reduction of the number of EF molecules at the thermal decomposition in the vessel is

$$\frac{\partial N}{\partial \tau} = -fN, \tag{1}$$

where τ is a residence time and $f \geqslant 0$ is some nonnegative function. Eq. (1) reminds the main law of radioactive decay, however here the function f has a more complicated form. Integration of Eq. (1) gives

$$\ln \frac{N}{N_0} = -\int_{\tau_0}^{\tau} f \, dt.$$

Definition. The function

$$\Psi = 1 - \frac{N}{N_0} = 1 - \exp\left(-\int_{\tau_0}^{\tau} f \, dt\right) \tag{2}$$

is called a local decomposition degree of EF (LDDEF). The function $0 \leqslant \Psi < 1$ defines a local activity of the EF decomposition.

A mathematical model of a cooling system of a combustion chamber wall of an aircraft engine requires an equation for computation of LDDEF. In order to obtain this equation, we divide both sides of Eq. (1) on N_0

$$\frac{\partial}{\partial \tau}\left(\frac{N}{N_0}\right) = -f\frac{N}{N_0}. \tag{3}$$

Eq. (2) gives

$$\frac{N}{N_0} = 1 - \Psi,$$

and Eq. (3) can be rewritten as

$$\frac{\partial \Psi}{\partial \tau} = (1 - \Psi)f, \tag{4}$$

where $\Psi = \Psi_0$ at $\tau = \tau_0$ (i.e. in the reference time τ_0).

For purpose of convenience, we introduce an auxiliary function $\hat{\Psi} = \ln(1 - \Psi)$. There are different approaches for approximation of the right hand side function f of Eq. (4). The most popular approximation takes the Arrhenius form

$$f = A \exp\left(-\frac{E}{RT}\right), \tag{5}$$

where A (s^{-1}) and E (J/mole) are some empirical constants (which are different for different EF), $R = 8.318$ J/(kmol·K) is absolute gas constant and T is absolute temperature (K).

Using the approximation (5) and Eq. (4), the auxiliary function $\hat{\Psi}$ coupled with LDDEF as $\hat{\Psi} = \ln(1 - \Psi)$ can be computed by solving the problem:

$$\frac{\partial \hat{\Psi}}{\partial \tau} = -A \exp\left(-\frac{E}{RT}\right), \qquad \hat{\Psi}(\tau_0) = \hat{\Psi}_0. \tag{6}$$

Now we consider an adaptation of the problem (6) for computation of LDDEF in curvilinear channels of the cooling system. At first, we consider the EF flow between the parallel heated plates. Remember that τ in (6) is the residence time and it coincides with the physical time t only for motionless EF. However for EF flow between plates, the residence time τ depends on local speed and passed distance, i.e. it is possible to assume that

$$u = \frac{dx}{dt},$$

where u is a velocity component of EF flow in the axial direction (along plates). Accounting $dt = dx/u$, Eq. (6) can be rewritten as

$$\frac{\partial \hat{\Psi}}{\partial x} = -\frac{A}{u} \exp\left(-\frac{E}{RT}\right). \qquad \hat{\Psi}(\tau_0) = \hat{\Psi}_0. \tag{7}$$

Eq. (7) predicts that the most intensive thermal decomposition of EF takes place at high temperature and/or slow fluid velocity. Therefore application of the rectilinear channels in the cooling systems seems to be problematic because of the EF decomposition will take place mainly in the near wall region. It is clear that full usage of the endothermic cooling capacity can be possible only at uniform decomposition in the channel cross-sections.

Obtained Eq. (7) has the following disadvantages:

1) the turbulent flows are characterized by random fluctuations of velocity, pressure and temperature. As a result, the residence time computed by the Reynolds averaged values will be less than the time computed by instantaneous values. It is expected that the constants A and E in Eq. (7) should be functions of the Reynolds number;

2) Eq. (7) gives inaccurate prediction of LDDEF in near wall region. Really the non-slip conditions lead to

$$u \to 0 \Rightarrow \hat{\Psi} \to -\infty \Rightarrow \Psi \to 1,$$

i.e. full decomposition of EF on the heated walls is expected.

Computation of the residence time of the reacting medium in different technical devices is sufficiently difficult problem [9, 10, 11, 12]. The modern methods of the residence time computation require impressive computational works. Obtained results can be inaccurate for the engineer applications.

Let us rewrite Eq. (7) as

$$\rho u \frac{\partial \hat{\Psi}}{\partial x} = -\rho A \exp\left(-\frac{E}{RT}\right),$$

where ρ is FM density. It is easy to see that this equation is similar to convective "part" of some transport equation written in nonconservative form. It is expected that the equation for the function $\hat{\Psi}$ can be written as

$$\frac{\partial(\rho\hat{\Psi})}{\partial t} + \nabla\left(\rho\vec{V}\hat{\Psi}\right) = -\rho A \exp\left(-\frac{E}{RT}\right),$$

where t is physical time, $\vec{V}$ is a velocity vector and ∇ is the Hamilton operator. It is expected that this equation can be rewritten in the following general form

$$\frac{\partial(\rho\hat{\Psi})}{\partial t} + \nabla\left(\rho\vec{V}\hat{\Psi}\right) = \nabla\left(D_{\hat{\Psi}}\nabla\hat{\Psi}\right) - \rho f, \tag{8}$$

where the function f is taken from Eq. (1) and $D_{\hat{\Psi}}$ is a "diffusion" coefficient.

Boundary conditions for Eq. (8) are given by:

a) inlet (inlet Ψ is given)

$$\hat{\Psi}\Big|_{\text{inlet}} = \ln\left(1 - \Psi\Big|_{\text{inlet}}\right),$$

b) outlet

$$\frac{\partial\hat{\Psi}}{\partial n}\Big|_{\text{outlet}} = 0,$$

where n is outlet normal.

c) channel wall ($\tau = t$)

$$\frac{\partial\hat{\Psi}}{\partial t}\Big|_{\text{wall}} = -A \exp\left(-\frac{E}{RT_w}\right), \tag{9}$$

where T_w is the wall temperature.

Thermal decomposition of EF is non-stationary process: on each time layer first computed $\hat{\Psi}_w$ on the heated walls of the channel (9) and after $\hat{\Psi}$ is computed in the domain (8). Verification of the model requires large computationat efforts and now the simplified model based on assumption that $D_{\hat{\Psi}} = 0$ will be used for EF simulation. The simplified model has a stationary solution because of Eq. (8) does not use the boundary conditions on the heated walls in case $D_{\hat{\Psi}} = 0$.

Note that Eq. (4) makes it possible to predict the nonfailure operation time of the cooling system. Integration of Eq. (4) gives

$$\frac{1 - \Psi(\tau)}{1 - \Psi(\tau_0)} = \exp\left(-\int_{\tau_0}^{\tau} f(t, T)\, dt\right).$$

Assuming that $\Psi(0) = 0$ and $f(t, T) = const$, we have

$$1 - \Psi(\tau) = \exp\left(-\tau f(T)\right).$$

Let is $\Psi_{\text{max}}(\tau_{\text{max}})$ maximum permissible value of the LDDEF. If $1 \geqslant \Psi \geqslant \Psi_{\text{max}}$ then formation of solid deposits on the heated wall can be expected. This equation

$$1 - \Psi_{\text{max}} = \exp\left(-\tau_{\text{max}} f(T_{\text{max}})\right)$$

results in the estimation of the nonfailure operation time $\tau_{\max}$

$$\tau_{\max} = -\frac{\ln(1 - \Psi_{\max})}{f(T_{\max})}.$$

If $f(T)$ is taken as (5), finally we have

$$\tau_{\max} = -\frac{\ln(1 - \Psi_{\max})}{A\exp\left(-\dfrac{E}{RT_{\max}}\right)}.$$

2.2 Source term in energy equation

The energy equation accounting the endothermic reaction is written as

$$\frac{\partial(\rho i)}{\partial t} + \nabla\big(\rho\vec{V}i\big) = \nabla\big(\lambda\nabla T\big) - S, \tag{10}$$

where i is FM enthalpy. If the function f is taken from Eq. (1), the source term S depends on FM decomposition degree of and temperature T as follows

$$S = AB\rho\exp\left(\hat{\Psi} - \frac{E}{RT}\right),$$

where A and B (J/m^3) are some empirical coefficients depending on EF. The source term $S > 0$ accounts the extra cooling capacity arising at thermal decomposition of EF.

2.3 State equation of the fictitious medium

Thermophysical properties of EF (density ρ_{EF}, dynamic viscosity μ_{EF}, heat conductivity λ_{EF} and heat capacity $c_{p\,\mathrm{EF}}$) depend on the temperature and pressure, i.e. $\rho_{\mathrm{EF}}(P,T)$, $\mu_{\mathrm{EF}}(P,T)$, $\lambda_{\mathrm{EF}}(P,T)$, $c_{p\,\mathrm{EF}}(P,T)$. Then state equation of FM can be formulated by interpolation, for example

$$\rho_{\mathrm{FM}}(P,T,\hat{\Psi}) = \exp(\hat{\Psi})\rho_{\mathrm{EF}}(P,T) + \big(1 - \exp(\hat{\Psi})\big)\rho_{\mathrm{DP}}(P,T,\hat{\Psi}), \tag{11}$$

where $\rho_{\mathrm{DP}}(P,T,\hat{\Psi})$ is density of the decomposition products (DP).

2.4 Mathematical model of the conjugate heat transfer

The 3D mathematical model of the cooling system consists of the following equations:
1) for FM flow:
   a) continuity and momentum equations (Navier-Stokes equations),
   b) equations for $(k - \varepsilon)$–model of turbulence,
   c) energe equation with extra source term (10),
   d) state equation (in form of (11)),
   e) equation for computation of the decomposition degree (8) .
2) for the cooling system construction:
   a) heat conductivity equation.

The model coincides with standard model of the conjugate heat transfer at low temperatures ($T < 600$ K $\Rightarrow \Psi \to 0$).

3 NUMERICAL EXPERIMENTS

A panel of the cooling system for aviation ramjet engine is a rectangle plate manufactured from a high-temperature steel with an internal channel for EF supply. Fragment with Π-like channel will be named as a heat-exchange section. Fig. 2 represents the overall sizes of the typical heat-exchange section with the channel for EF supply. The cooling panel consisting of three heat-exchange sections is shown on Fig. 3.
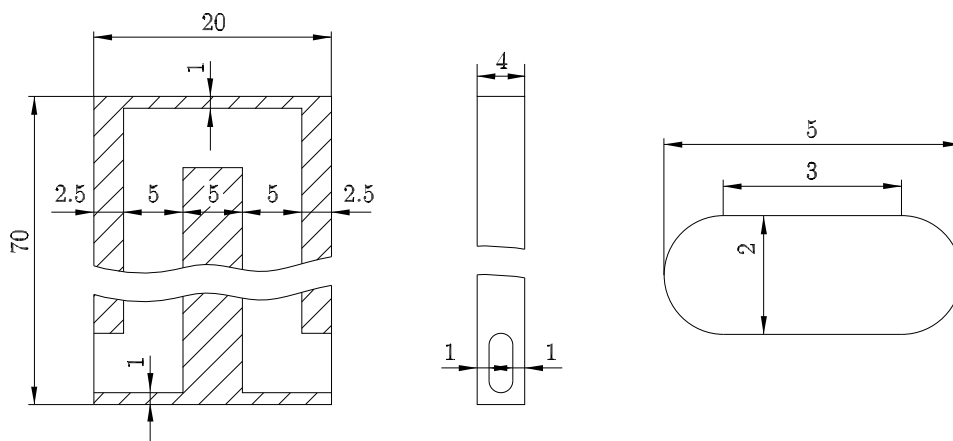

Figure 2: Geometry of the heat-exchange section with the internal channel for EF supply (all sizes are given in millimeters).
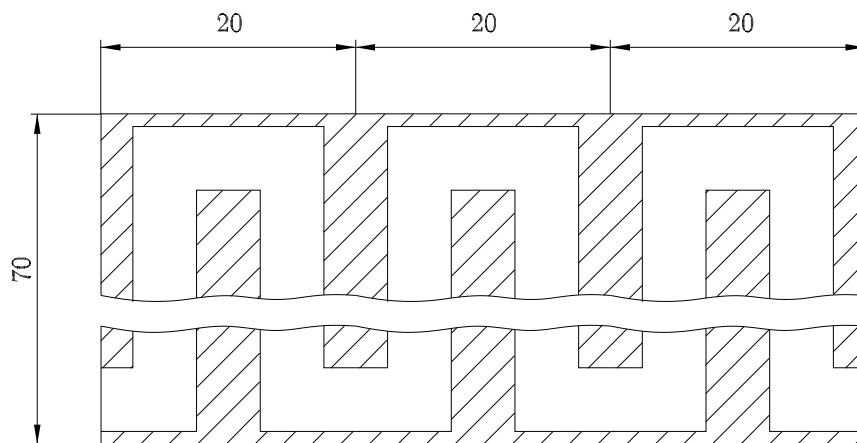
Figure 3: The cooling panel consisting of three heat-exchange sections (all sizes are given in millimeters).

Heat-insulated manifold equips the last heat-exchange section as shown on Fig. 4. The manifold is needed for the correct formulation of the outlet boundary conditions for momentum, energy, $(k - \varepsilon)$–equations and Eq. (9). It is assumed that zero Neumann conditions are given on the manifold outlet.

Unstructured grid in the panel (633047 control volumes in each section) and structured grid in the channel (191862 control volumes in each section) are generated for approximation of the basic partial differential equations (Fig. 5).

It is well known that roughness has strong influence on convective heat transfer in the channels (especially for small equivalent diameters). In our numerical experiments the uniform microroughness height is taken to be $4 \cdot 10^{-5}$ m.
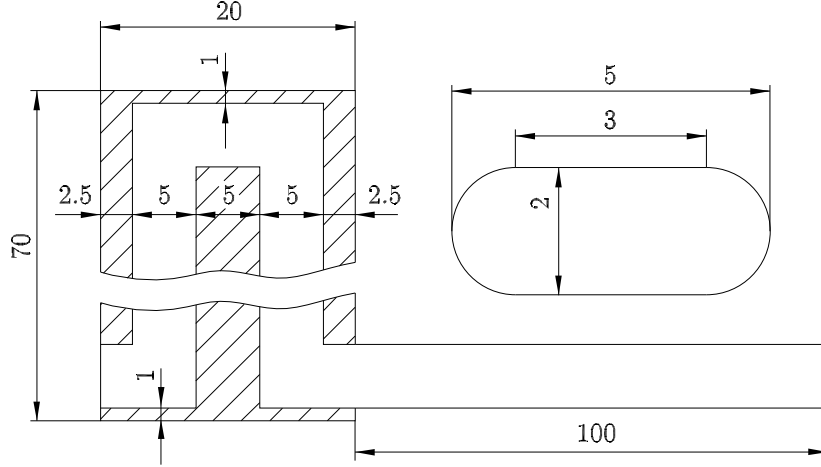

Figure 4: Last heat-exchange section and the heat-insulated manifold.

Pentane (C_5H_{12}) under supercritical pressure $p_0 = 5$ MPa is taken as the EF. Values of the empiric constants for the pentane are $E = 231268$ J/mole, $A = 1.75 \cdot 10^{12}$ c^{-1}, $B = 1.68 \cdot 10^6$ J/m^3. Inlet temperature of the pentane is $T_0 = 300$ K, mass flow rate is 0.0067 kg/s.

To analyze results of the computations, we use the following parameters:
1) maximum temperature ($T_{\max}$) and maximal LDDEF ($\Psi_{\max}$)

$$T_{\max} = \max_{\Omega_{ijk}} T_{ijk}, \qquad \Psi_{\max} = \max_{\bar{\Omega}_{ijk}} \Psi_{ijk}, \tag{12}$$

where Ω_{ijk} and $\bar{\Omega}_{ijk}$ are used computational grids in metal part of the panel and channel, respectively.
2) mass-averaged flow temperature $\langle T_f \rangle$ and mass-averaged LDDEF $\langle \Psi \rangle$

$$\langle T_f \rangle = \frac{\int\limits_s \rho u T_f \, d\sigma}{\int\limits_s \rho u \, d\sigma}, \qquad \langle \Psi \rangle = \frac{\int\limits_s \rho u \Psi \, d\sigma}{\int\limits_s \rho u \, d\sigma}, \tag{13}$$

where s is an area of the channel cross-section and u is velocity component.
3) mass-averaged LDDEF $\langle \bar{\Psi} \rangle$ in the manifold outlet (Fig. 4)

$$\langle \bar{\Psi} \rangle = \frac{\int\limits_m \rho u \Psi \, d\sigma}{\int\limits_m \rho u \, d\sigma}, \tag{14}$$

where m is an area of the outlet cross-section of the manifold.

Goal of the numerical experiments is to computational study the cooling panel from point of view of intensification heat transfer, minimization of hydraulic resistance and maximum usage of the endothermic effect at EF decomposition. Some EFs have tendency to coke deposit
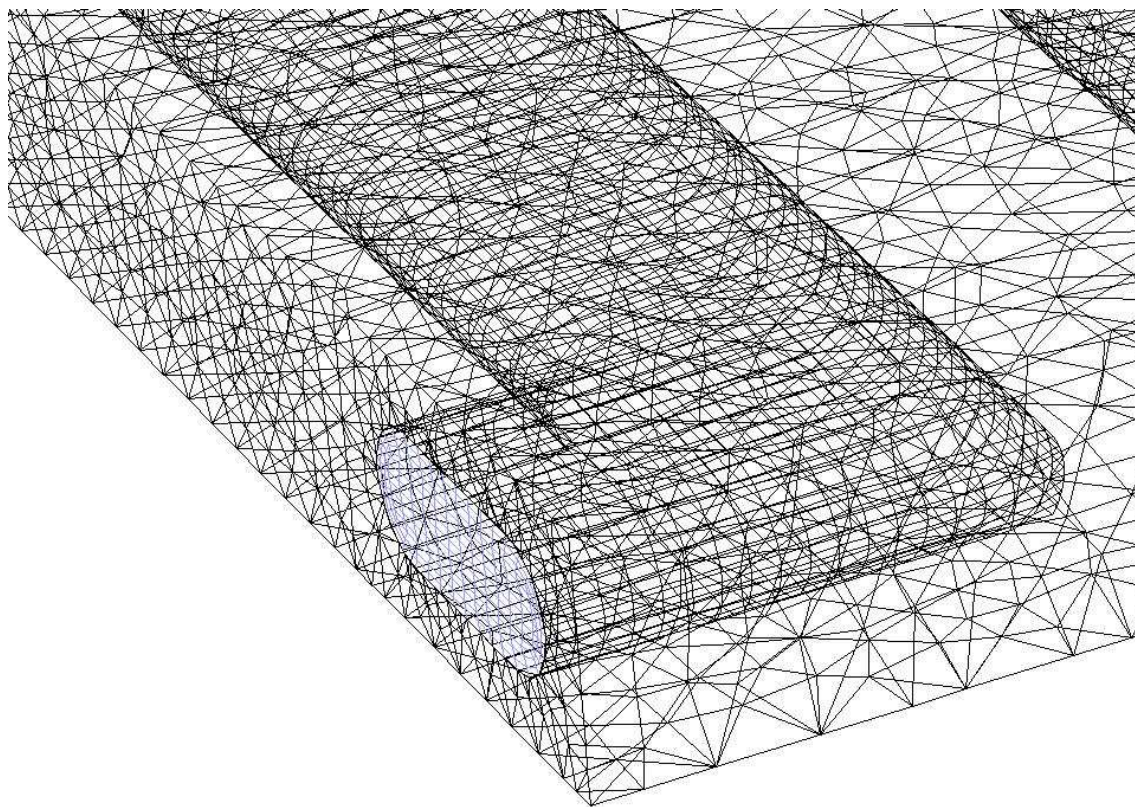
Figure 5: Computational grid in the cooling panel.

formation on overheated channel walls. Layer of the solid coke deposits results in additional heat resistance and reduces the cooling system efficiency. To overcome this problem, operating conditions of the cooling system should guarantee that maximum LDDEF is limited by some value, for example $\Psi_{max} < 0.8$.

We summarize the main features of the cooling system:

a) Near inlet region. Heat of cold EF leads to remarkable change of their thermal properties (density, viscosity, heat conductivity etc.). If the channel cross-sectional area is the same, reduction of EF density results in increase of hydraulic resistance. The channel configuration should ensure intensification of convective heat transfer without unpractical hydraulic losses.

b) Near outlet region. EF is overheated up to their thermal decomposition. The decomposition starts in the channel subdomains with high temperature and high residence time (or small linear velocity), i.e. it is expected that the decomposition will take place in small overheated sublayer in near wall region. As a result, all endothermic cooling capacity of EF cannot be used in such system because of coke deposit hazard near walls and cold flow core. In addition, the channel configuration should ensure sufficient residence time for required decomposition value.

It is expected that the channel configuration shown on Fig. 3 results in continuous mixing of EF flow. In near inlet region the mixing leads to the convective heat transfer intensification and in outlet region the mixing leads to temperature balance in channel cross-sectional area and increase of residence time for needed decomposition value. Disadvantage of the cooling system is high hydraulic resistance as compared with straight channels.

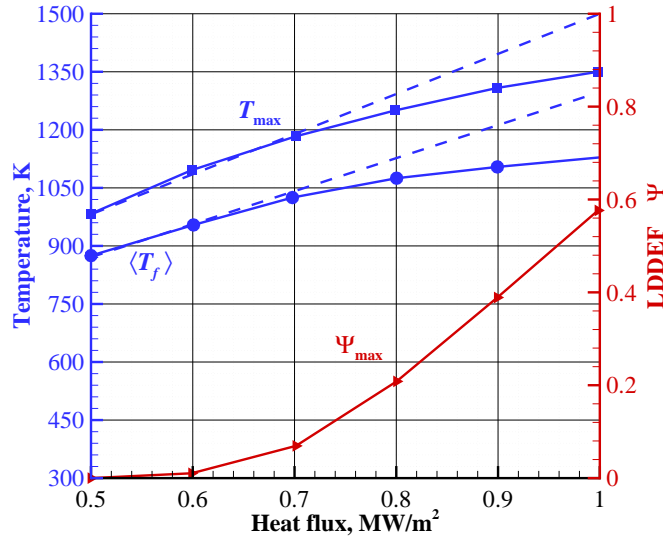Fig. 6 represents influence of the pentane decomposition on the outlet temperature of the

Figure 6: Influence of the endothermic effect on temperature of twenty sectional panel of the cooling system: without (dashed line) and with (solid line) taking the pentane decomposition into account at uniform heat flux.

cooling panel at different values of heat flux. Here T_{max}, Ψ_{max} and $\langle T_f \rangle$ are given by (12) and (13) in outlet section, respectively. Maximum value of LDDEF $\Psi_{max} \approx 0.6$ predicts absence of solid deposit formation on the channel surface under these conditions.

Results of numerical simulation of the heat transfer in twenty sectional panel of the cooling system are given in Table 1. The table represents maximal values of LDDEF Ψ_{max} (12) and temperature T_{max} (12), mass-averaged outlet values of LDDEF $\langle \bar{\Psi} \rangle$ (13) and EF temperature $\langle T_f \rangle$ (13) and mass-averaged outlet values of LDDEF $\langle \bar{\Psi} \rangle$ (14) in the outlet manifold (Fig. 4) at different heat fluxes. Note that the hot EF continues to decompose in the outlet heat-insulated manifold: $\langle \Psi \rangle < \langle \bar{\Psi} \rangle$. This fact should be accounted at the cooling system designing since the solid depositions formation in the outlet manifolds can take places at high values of LDDEF.

Fig. 7 shows distribution of temperatures, LDDEF, averaged Reynolds number and averaged pressure in the panel at $q = 1$ MW/m^2. In spite of strong change of the pentane thermal properties, pressure drop is 0.5 MPa (from inlet pressure 5 MPa downto outlet pressure 4.5 MPa). Computational results predicts that the panel (size 0.07×0.4, coolant (pentane) mass flow rate is 0.0067 kg/s, $T_{inlet} = 300$ K, $p_{inlet} = 5$ MPa) can be used for the combustion chamber

Heat flux	Two last sections		Outlet		Manifold
q, MW/m^2	Ψ_{max}	T_{max}, K	$\langle \Psi \rangle$	$\langle T_f \rangle$, K	$\langle \bar{\Psi} \rangle$
0.5	0.00	983.75	0.00	868.71	0.00
0.6	0.01	1088.98	0.01	953.04	0.01
0.7	0.07	1181.17	0.04	1025.02	0.05
0.8	0.21	1248.60	0.15	1070.53	0.17
0.9	0.39	1300.98	0.31	1098.90	0.34
1.0	0.58	1349.14	0.48	1125.04	0.52

Table 1: Result of the heat transfer simulation in twenty sectional panel of the cooling system.
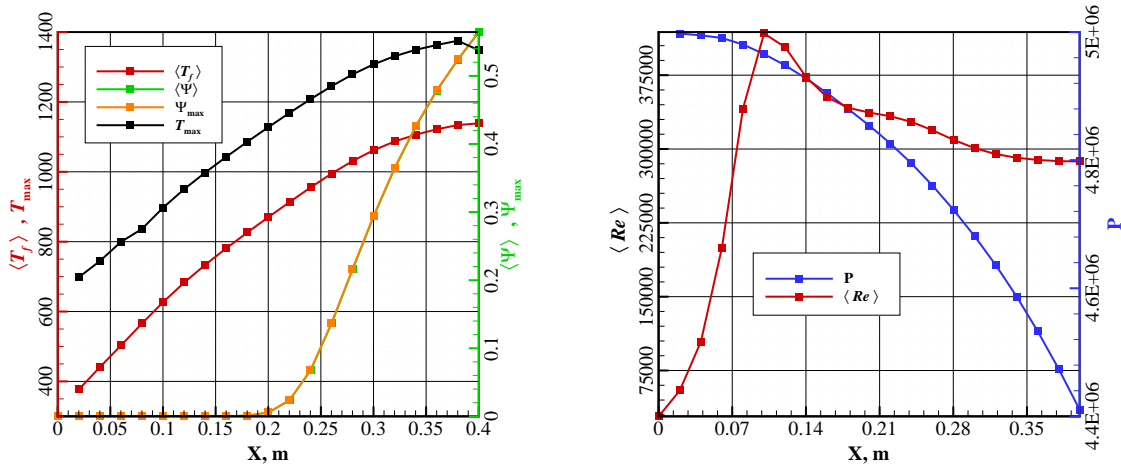
Figure 7: Distribution of LDDEF Ψ and temperature T (K) (left), Reynolds number Re and pressure p (Pa) (right) in twenty sectional panel of the cooling system at heat flux $q = 1$ MW/m^2.
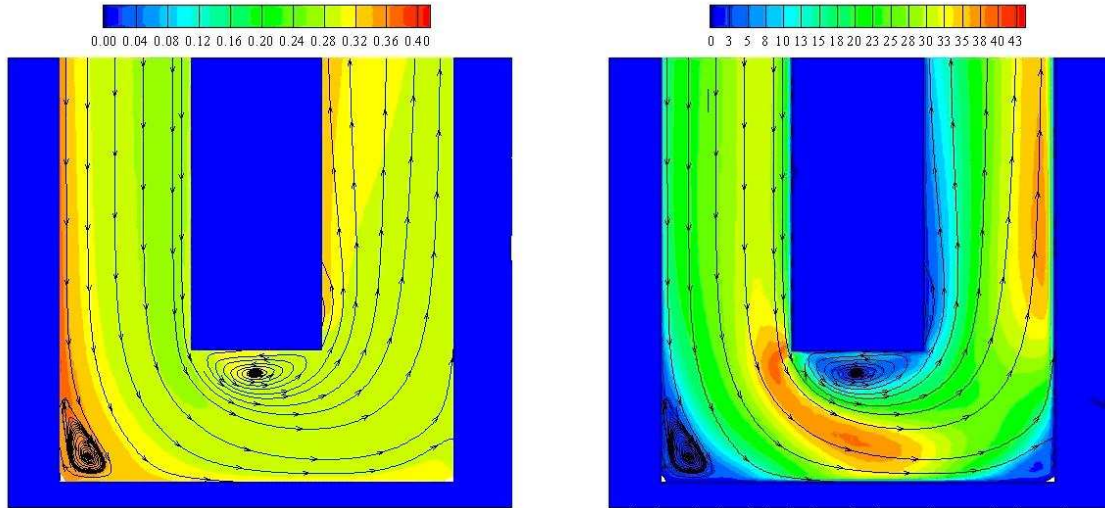

Figure 8: Distribution of LDDEF Ψ (left) and velocity modulus (m/s) (right) on boundary between penultimate and last heat exchange sections at heat flux $q = 1$ MW/m^2.

protection.

Fig. 8 represents the planar distribution of LDDEF and absolute value of EF velocity between penultimate and last heat exchange sections ($q = 1$ MW/m^2). The panel geometry gives intensive EF mixing in the channel. As a result, almost uniform EF temperature distribution in the channel cross-section is observed. In this case thermal decomposition of EF depends only on the local velocity. Recirculating zones lead to increase EF residence time and LDDEF [13].

4 FUTURE WORKS

Proposed mathematical models have advantages in computational efforts. The model allows simulate physical and chemical process in multidimensional reacting EF flows and burning in the combustion chamber in coupled manner. However real hydrocarbon fuels consist of many compounds and their thermal decomposition has complex multistage nature. Detailed mechanism of thermal decomposition of simple hydrocarbon fuels consists of many elementary reac-
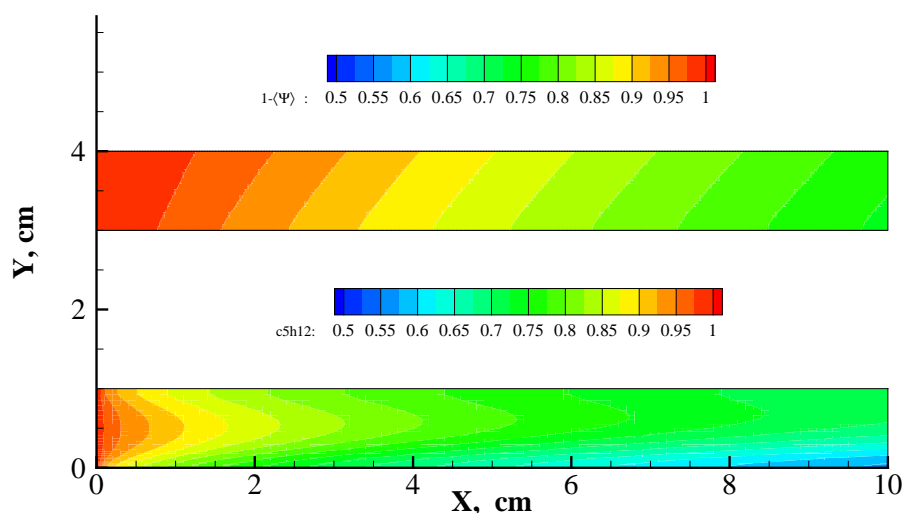
Figure 9: Mass fraction of pentane, laminar flow between parallel plates at $T_{\max} = 700$ K: brutto-approximation (upper figure) vs. detailed kinetics of the decomposition (lower figure).

tions. As a result, sufficiently accurate mathematical models can include thousands equations and it difficult to use for practical computations. The most promising approach is reduction to the simplified description. The simplified model should describe such the main features of full model as heat sources and outlet substances concentrations. Fig. 8 represents comparison of results obtained by using full model (more than 1000 reactions and 200 components [14]) and proposed model. Fig. 8 demonstrates simulation of 2D laminar flow between parallel plates, lower plate is heated and upper plate is heat heat-insulated. Inlet temperature is close to temperature of the decomposition start (700 K). Average cross-sectional values of the decomposition degree are similar to each other (maximum difference is no more than 10%), but their spatial distributions are differ.

Following development of proposed model is hybrid approach based on chain-radical mechanism of the thermal destruction and global brutto-correlations for components of the reacting system.

ACKNOWLEDGEMENT

5   CONCLUSIONS

3D mathematical model have been proposed to simulate the scramjet active cooling system and to determine the mixture composition at the cooling channel outlet. To minimize the computational efforts, the one-step pyrolytic reaction mechanism has been used for the pentane decomposition. As a result, it is possible to compute physical and chemical processes in the combustion chamber and its cooling system in coupled manner. At present time a mathematical model with more accurate description of EF decomposition based on complete detailed mechanism is developed.

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