EFFECTS OF THE ELECTROMAGNETIC FIELDS TO COKE DEPOSIT FORMATION AT ENDOTHERMIC FUEL FLOWS IN HEATED CHANNELS OF THE HIGH SPEED ENGINES

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Abstract

The paper represents the mathematical model of hydrocarbon fuel flows with taking into account the coke deposit formation on the heated walls of cooling systems of aeroengines. This model can predict an effect of a weak electromagnetic field on intensity of coke deposit formation. It is shown the effect of the electric field (E = 0.1...100 V/m) on coke precursors (high molecular products of fuel oxidation) deposition at different wall temperatures in channels.

Nomenclature

ρ density, kg/m^3;

$\mathbf{U}$ velocity vector, m/s;

p pressure, Pa;

τ viscous stress tensor, Pa;

q   volume charge, C;

h   enthalpy, J/m;

T   temperature, K;

$\mathbf{F}$ Lorentz force, N;

m_r molecular weight of the neutral components in the impulse exchange, kg/mol;

v_{ir}'', v_{ir}' stoichiometric coefficients of the reactants and the reaction products

Y_j mass concentration of the component, kg/kg;

J_j specific mass flux, $kg/(m^2 s)$;

J_j^c mass diffusion coefficient of the component in the mixture, m^2/s;

Sc_t turbulent Schmidt number;

U_d ion drift velocity, m/s;

n_e concentration of the electrons, m^{-3};

S source term accounted the chemical reactions, $m^{-3}s^{-1}$;

μ_e electron mobility, $m^2/(V \cdot s)$;

D_e diffusion coefficient of the electronic components, m^2/s;

φ electric field potential, V.

Introduction

Coke deposits on the heated surfaces of fuel system of high speed engine lead to increase of the manifold hydraulic friction and wall thermal resistance[1]. As a result, a overheating of the manifold is expected. One of the main thermochemical reason of the coke deposit formation under supercritical pressure is an oxidation of molecules of unstable fuel components by dissolved oxygen. It results in generation of intermediate active reaction products (free radicals)[2]. Interaction of the radicals and molecules of the fuels give rise to the coke deposits[3].

The deposit rate depends on many factors, the main of them are the fuel and wall temperatures, pressure, fuel speed and properties of the wall surface (roughness and chemistry). Also the deposit rate depends strongly on the material of the manifold walls having catalytic influence of the fuel oxidation.

The reliable operation of fuel systems of aircraft engines depends substantially on the processes occurring in a fuel. For example, addition of the surface-active substances to a fuel can reduce an engine reliable operation in a several times[11]. The most dangerous phenomenon is a coke deposit formation on internal surfaces of

fuel manifolds. The coke deposits change the physical and chemical properties of channel surfaces that effect on hydrodynamics and heat transfer. Thermal oxidation of a heated fuel results in formation of the intermediate products (radicals and neutral compounds) of different molecular mass, i.e. electrically neutral fuel transforms into a mixture of the electrically charged ionic components and radicals[2]. These components have different mobility and it can be controlled by the electromagnetic fields. External electromagnetic fields can result in spatial separation of the charged components and alteration of the equilibrium values of the constants of elementary chemical reactions.

Some experimental results about action of the electromagnetic fields on the coke deposits are given in[4], but there are not 3D mathematical models of the coke formation under influence of the electromagnetic fields.

Fig. 1 represents scheme of the process and the fuel cooling channel geometry. Electrodes are installed in the middle part on the lower and upper walls of the channel ($200 \times 10 \times 1$ mm). Distance from the channel inlet to the electrode is 90 mm, a length of the electrodes is 10 mm, i.e. the length is small for study of the local effect of the electromagnetic field on the coke deposit in the domain.

1. Mathematical model

Fig.2 shows the general scheme of the algorithm for solving the governing equations of the mathematical models. The algorithm consists of five blocks starting from Reynolds equations down to transport equation for the electronic components. These blocks are coupled by velocity, pressure, temperature and source terms. In the first block well known method SIMPLEC is used for coupling pressure and the mixture velocity. Many partial differential equations

had been reduced to general form of the transport equation. Control volume method is used for the approximation of the PDEs on unstructured hexahedral grid. The number of the control volumes is $\sim 10^6$. Sets of linearized discrete equations are solved by Generalized Bi-Conjugate Gradient Stabilized with incomplete LU factorization.
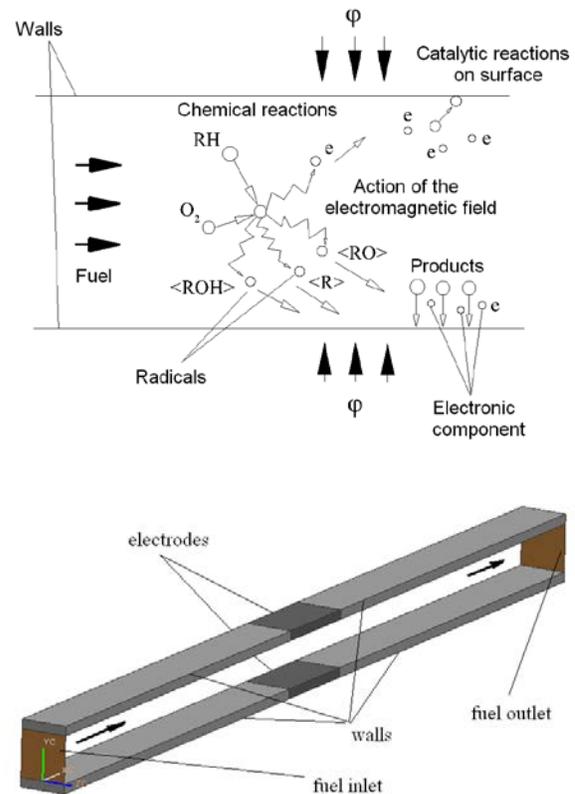

Fig.1. Scheme of the process of the fuel oxidation under the electromagnetic field in the channel.

Temperature, composition of the mixture, parameters for turbulent flows and flow consumption are known for the inlet channel section. "Smooth" boundary conditions are posed in the outlet section. It is assumed that the chemical reactions on wall surface does not affect on the geometry and heat conditions of the channel walls.

1.1 Fuel model

The turbulent fluid flow is described by Reynolds equations for the multicomponent mixtures and Spallart-Almaras turbulence model[5]. The averaged Navier-Stokes equations take the form[6]:

Reynolds equations and Spallart-Almaras turbulence model for the multicomponent medium

Transport equations for the neutral components (products and reagents of the chemical reactions)

Transport equations for the charged components (radicals) and solutions of ordinary differential equations of the chemical kinetics

Energy equation for the mixture (in form of the full enthalpy) and for temperature of the electronic component

Equation of electrostatic field in form of potential and transport equation for the electronic component
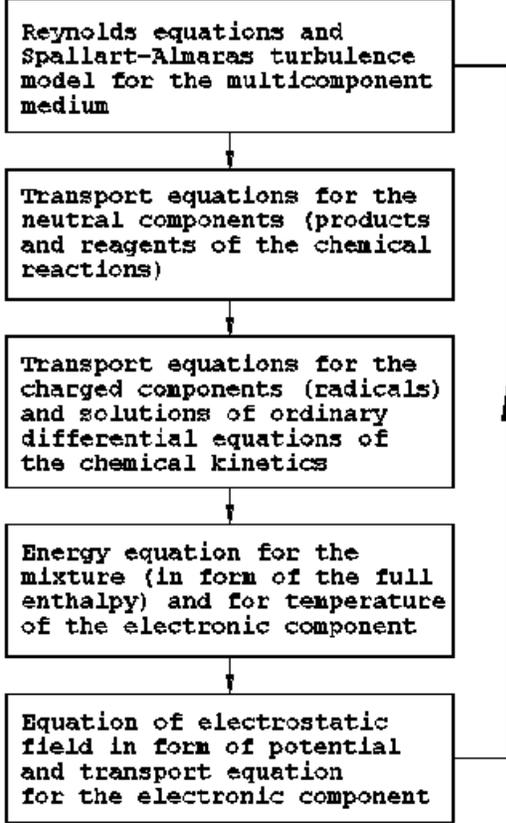
Fig.2. Iterative solver of the governing equations.

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{U}) = 0, \qquad (1a)$$

$$\frac{\partial(\rho \mathbf{U})}{\partial t} + \nabla(\rho \mathbf{U} \times \mathbf{U}) = -\nabla p + \nabla \tau + \mathbf{F}, \qquad (1b)$$

$$\mathbf{F} = q\mathbf{E} + \mathbf{J} \times \mathbf{B}, \qquad (1b)$$

$$\frac{\partial(\rho C_p \mathrm{T})}{\partial t} + \nabla(\rho \mathbf{U} C_p \mathrm{T}) = \nabla(\lambda \nabla \mathrm{T})$$
$$+ \sum_i J_i C_{pi} \nabla \mathrm{T} + Q - \sum_{r=\text{elastic}} \varepsilon_r \dot{\omega}_r + \sum_{r=\text{ions}} \varepsilon_r \dot{\omega}_r. \qquad (1c)$$

The right side of the energy equation (1c) contains the source terms associated with elastic collisions of the electronic component, ohmic heating of the ion component, the thermal effect of

volumetric and surface reactions. Heat generation due to the non-electronic reactions and the elastic electron collisions (the last two terms in the abovementioned equation) is

$$\varepsilon_r = \begin{cases} \sum_i (v''_{ir} - v'_{ir}) h_i, & \text{for the ions,} \\ 2\dfrac{m_e}{m_r} e\left(\bar{\varepsilon}_r - \dfrac{3}{2}T_g\right), & \text{for the electrons} \end{cases} \qquad . (2)$$

The source term (2) associated with the interaction between the ionic and the neutral components can be written as

$$\dot{Q} = \sum_{q_i > 0} q_i n_i \mu_i E \cdot E$$

To determine the concentrations of the ionic and the neutral components, the ion drift is accounted by the equation

$$\frac{\partial}{\partial t}(\rho Y_j) + \nabla \cdot (\rho \upsilon Y_j) = -\nabla \cdot J_1,$$

$$J_j = -\left(\rho D_{j,M} + \frac{\mu_t}{Sc_t}\right) \nabla Y_j + \rho U_d Y_j + J_j^c, \qquad (3)$$

where the turbulent Schmidt number is $Sc_t = 0.7$.

In eq. (3) linear approximation is assumed for the ion drift velocity

$$U_d = \left(q_i \mu_i - \sum_j q_j \mu_i Y_j\right) E.$$

Langevin formula is used for the computation of the ion mobility:

$$\mu_{ij} = \frac{0.00013853}{\sqrt{\alpha'_j m_r}},$$

where m_r is the component mass, α'_j is the so-called polarizability volume (in A^3) associated with a dielectric constant of the component by the Clausius-Mossotti[7]:

$$\frac{\varepsilon - \varepsilon_0}{\varepsilon + 2\varepsilon_0} \cdot \frac{\grave{I}}{\rho} = \frac{4\pi N_A \alpha'}{3}.$$

Here $\grave{I}$ is molar mass and N_A is Avogadro number, respectively.

1.2. Electromagnetic field model

The equation for electric (φ) and vector potential (A) with

charged components in computational domain is used for determination of the strength distribution of electric and magnetic fields[8]:

$$-\nabla \varepsilon \nabla \varphi = e\left(\sum_i q_i n_i - n_e\right)$$

1.3. Model of a charged mobile phase

Motion of the electrons can be predicted by the transport equation:

$$\frac{\partial n_e}{\partial t} + \nabla \tilde{A}_{\dot{a}} = S,$$

where

$$\tilde{A}_{\dot{a}} = \mu_e n_e \nabla \varphi - D_e \nabla n_e.$$

Electron mobility and diffusion can be computed using the two-particle distribution function of the probability density of the electron energy by the following formulas (used Maxwell energy distribution):

$$\mu_e = \frac{1}{n_e}\int_0^\infty \sqrt{\varepsilon} D_r(\varepsilon)\frac{\partial f_0}{\partial \varepsilon}d\varepsilon,$$

$$D_e = \frac{1}{n_e}\int_0^\infty \sqrt{\varepsilon} D_r(\varepsilon) f_0(\varepsilon) d\varepsilon,$$

$$\overline{n}_e = \int_0^\infty \sqrt{\varepsilon} f_0(\varepsilon) d\varepsilon,$$

where ε – kinetic energy of the particles, $\overline{n}_e$ – the electron density, $f_0(\varepsilon)$ – first term in the expansion of f, $D_r(\varepsilon) = \lambda v_e/3$ is the diffusion coefficient with average electron free path $\lambda = v_e/v_m(\varepsilon)$, where the electron collision frequency is given by[9,10]

$$v_m(\varepsilon) = v_e(\varepsilon)\left\{\sum_s n_s\left(\sigma_{el}^s(\varepsilon) + \sigma_{inel}^s(\varepsilon)\right) + n_e\frac{\sigma_{em}(\varepsilon)}{\gamma_E}\right\}.$$

Here s is the index of the neutral component, n_s – the density, σ_{el}^s is elastic momentum transfer cross section, $\sigma_{inel}^s(\varepsilon)$ is the inelastic momentum transfer cross section, $\gamma_E = 0.544,$ and $\sigma_{em}(\varepsilon)$ is the momentum transfer cross section for the electron-ion interactions

$$\sigma_{em}(\varepsilon) = -\frac{\pi}{2(e\varepsilon)^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \ln\left(\frac{n_e e^3}{144\varepsilon_0^3\pi^2 T_e^3}\right). \quad (4)$$

Temperature of the electron components (T_e) satisfies to the equation

$$\frac{3}{2}\frac{\partial}{\partial t}(n_e T_e) + \nabla\left(\frac{5}{2}T_e\Gamma_e - \chi\nabla T_e\right) = .$$
$$= P - n_e\sum n_r k_r \varepsilon_r. \quad (5)$$

First term in the right side of the eq. (5) corresponds to the total effects of the processes with the absorption of energy by electrons (Joule P_J and inductive heating P_I)

$$P_J = J_e E = e\tilde{A}_e\nabla\varphi,$$

$$P_I = 0.5\, real(\delta)\omega^2\left|\tilde{A}\right|^2,$$

$$P_{ex} = \frac{2A\frac{1}{v^2}\iiint|J_e E|\iiint u_{e,mean}dV}{Lv_m},$$

where the upper wavy line marks the complex resistance and magnetic potential, respectively, $real(\delta)$ means the real part of δ. The complex resistance is computed as

$$\tilde{\sigma} = \frac{\varepsilon_0\omega_e}{v_m + i\omega},$$

where ε_0 is the electric constant, v_m – the electron collision frequency, $i = \sqrt{-1}$ – the imaginary unit, ω – inductive frequency. Natural frequency of the electronic component is

$$\omega_e = \sqrt{\frac{e^2 n_e}{\varepsilon_0 m_e}}.$$

Without reflection the electron flux normal to the wall ($\tilde{A}_{e,n}$) is written as

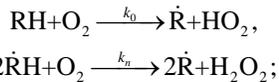$$\tilde{A}_{e,n} = 0.25 n_e\sqrt{\frac{8k_B T_e}{\pi m_e}} - \theta\sum_i q_i\tilde{A}_{i,n},$$

where q_i, $\tilde{A}_{i,n}$ are a single charge and mass flow of ith component.

It is assumed the thermophysical properties of the neutral component of fuel depend only on the temperature.

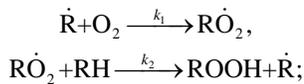### 1.4 Model of the coke deposit formation
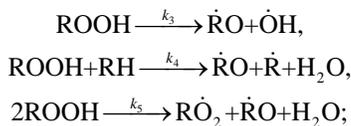
Liquid-phase oxidation of a hydrocarbon fuel by

the dissolved oxygen takes place at temperatures T < 550 K. Homogeneous laminar (Re ~ 1000) and turbulent regimes (Re > 4000) are considered. Value of pressure P ~ 5 MPa corresponds to the conditions in fuel systems of modern aviation engines. Kinetic model of the coke deposit formation is based on assumption of the radical-chain mechanism with degenerated chain branching[11]. This model is valid for small oxidation degree. Interaction of the hydrocarbons and dissolved oxygen leads to the chain formation. The radicals are generated slowly in absence of the initialize additions. As a rule, one of the stages of liquid-phase oxidation of a hydrocarbon fuel is the hydroperoxide formation. The hydroperoxide can decompose in O-O link and it is the reason of the additional chain origin.
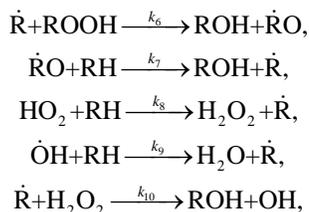
The chains origin:

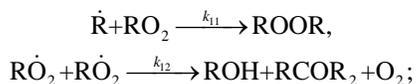$$RH+O_2 \xrightarrow{k_0} \dot{R}+HO_2,$$

$$2\dot{R}H+O_2 \xrightarrow{k_n} 2\dot{R}+H_2O_2;$$

Continued chains:

$$\dot{R}+O_2 \xrightarrow{k_1} R\dot{O}_2,$$

$$R\dot{O}_2+RH \xrightarrow{k_2} ROOH+\dot{R};$$

Degenerated chains branching:

$$ROOH \xrightarrow{k_3} \dot{R}O+\dot{O}H,$$

$$ROOH+RH \xrightarrow{k_4} \dot{R}O+\dot{R}+H_2O,$$

$$2ROOH \xrightarrow{k_5} R\dot{O}_2+\dot{R}O+H_2O;$$

Continued chains with the secondary products:

$$\dot{R}+ROOH \xrightarrow{k_6} ROH+\dot{R}O,$$

$$\dot{R}O+RH \xrightarrow{k_7} ROH+\dot{R},$$

$$HO_2+RH \xrightarrow{k_8} H_2O_2+\dot{R},$$

$$\dot{O}H+RH \xrightarrow{k_9} H_2O+\dot{R},$$

$$\dot{R}+H_2O_2 \xrightarrow{k_{10}} ROH+OH,$$

Bimolecular chain breaking in the volume:

$$\dot{R}+RO_2 \xrightarrow{k_{11}} ROOR,$$

$$R\dot{O}_2+R\dot{O}_2 \xrightarrow{k_{12}} ROH+RCOR_2+O_2;$$

Chains breaking on the wall:

$$\dot{R} \xrightarrow{k_w} , \dot{R}O \xrightarrow{k_w} , R\dot{O}_2 \xrightarrow{k_w} , \dot{O}H \xrightarrow{k_w} ,$$

$$HO_2 \xrightarrow{k_{w.}} , H_2O_2 \xrightarrow{k_w}$$
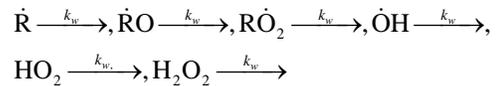
All radicals are labeled by a point over the characters in the abovementioned formulas. In addition, stoichiometrical coefficients of the electronic component are not given. Reaction constants are taken from[1]. High molecular products (HMP) similar to the products of a volumetric recombination of radicals (alcohols ROH, ketones R-R, aldehydes ROOR) are formed on the walls due to a bimolecular recombination of radicals. For reason of simplicity it is assumed that the first three radical-chain terminal reactions on a wall have the bimolecular nature and its lead directly to the formation of coke precursors. In addition, deactivation of an internal surface of a channel wall is not accounted in the computations. Really a part of HMP is adsorbed from a volume and polymerization of HMP should be accounted on walls.

Nevertheless, despite the considerable simplification in the kinetics of the coke deposit formation the proposed mathematical model contains the main stages of the deposits formation and this model can be used for analysis of the dynamics of the coke precursor formation.

2. Results of numerical simulation

The mathematical model is applied for computations of main characteristics of fuel flow in the channel. Fig. 3 (up) shows the field of electric potential and the profile of the axial velocity in the longitudinal section. Computational values are marked by a thin solid line; the data is given for t > 3600 sec. It is clear that a formation of discrete charged phase in a form of electrons and ions under the given conditions does not affect on the

global distribution of tension. Axial velocity in cross-section of the electrodes has a steady-state turbulent profile.

Fig. 3 (down) represents the field of HMP (more precisely: a sum of the mass fractions of alcohols ROH and aldehydes ROOR formed in the channel). In addition, this figure shows a profile of the mass concentrations across the channel along the middle line. Main fraction of HMP is formed in a boundary layer near the walls and a characteristic value of the fraction for the given time is 10^{-6} kg/kg.
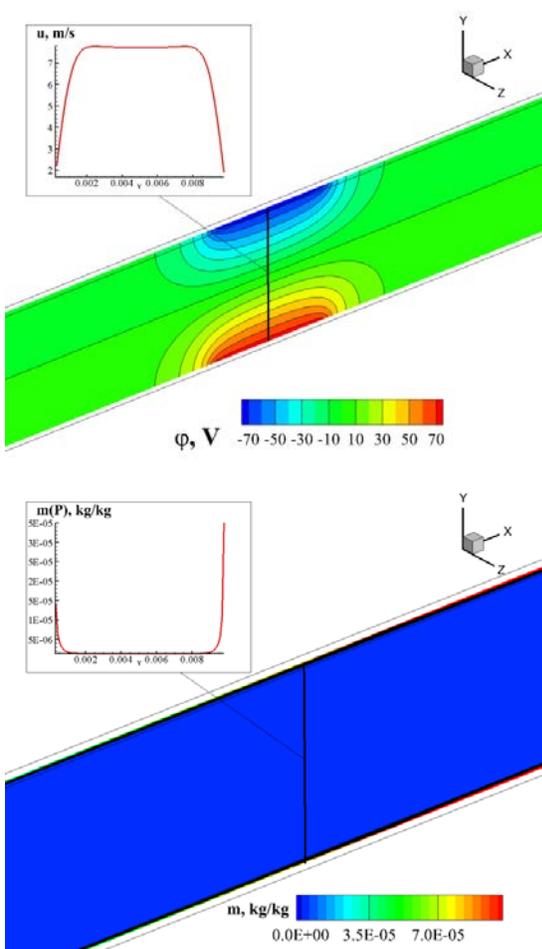
Fig.3. The electric potential and the profile of the axial velocity (up), the mass fraction of HMP and the profile (down) for fragment of the longitudinal median section of the channel: Re = 4000, Δφ=150 B, qw = 0, Tin = 600 K

Fig. 4 shows the distributions of the cross-averaged molar concentrations of the chemical components along the channel: radicals, intermediate products (R), HMP (alcohols and aldehydes (P)) and molecular oxygen (O_2). Data are shown for 20 equally-spaced cross-sections of the channel. Relative concentration of the HMP for time t = 3600 sec at distances up to X/h < 5...10 is small enough, where h is the channel width. These results correspond to experimental data for the oxidation in steel tube[11].
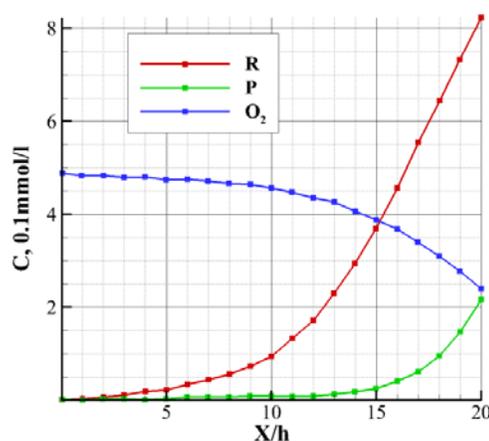

Fig. 4. Averaged concentrations of intermediate products (R), HMP of the alcohols and aldehydes (P) and oxygen O2 along the channel length: Re = 4000, Δφ=0 B, q_w = 0, Tin = 600 K

Fig. 5 shows the molar concentration of the products formed at bimolecular break of the radical chains on the wall: the total concentration of ketones, alcohols and aldehydes for different wall temperatures Tw (left) and various the potential difference applied to the electrodes (right). It is easy to see that mass of deposed HMP strongly depends on the wall temperature and weakly depends on the electric field. Domain of the deposed HMP is limited to 2-5 channel widths. The maximum deviation of the molar concentration (applicable

electromagnetic field Δφ=150 V) as compared with a zero potential difference is 25%.

Conclusion

Mathematical model for computation of a coke deposit formation on heated walls of a rectangular channel has been developed. This model based on Navier-Stokes equations and Maxwell equations (in the form of equations for the electric and magnetic potentials). Radical-chain mechanism of liquid-phase oxidation of hydrocarbon fuels is used for description of chemical reactions.
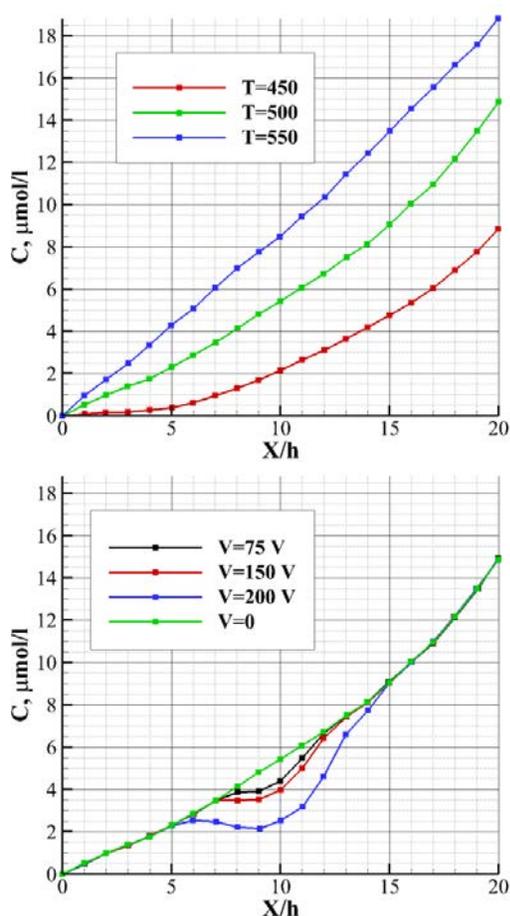
Results of computations show the wall temperature in the range 350 < T_w < 600 K has impressive influence on a coke deposit behavior (up to 50% of the deposit mass in the typical cross sections). The influence of the electric field in the given conditions is less in general, but the local effect of the potential difference to mass of the coke precursors is high: at potential difference between the electrodes of 100 V are approximately in 2.5 times.

The computational results have satisfactory accuracy for engineer applications. However, taking into account complex nature of coke deposit formation the model will be tested carefully using various experimental data.

Fig.5. Mass of coke precursors along the channels for different temperature (up) and the potential difference between the electrodes (down): Re = 4000,Tin = 400 K, t=3600 c.

References
1. Taylor W. Development of High Stability Fuel. Exxon Report. 1975. NGRV 13 GAH F.75. 326 p.
2. Emanuel N.M., Zaikov G.E., Mayzus Z.K. Role of the Environment in the Radical-Chain Oxidation Reactions of the Organic Compounds. Moscow, Nauka, 1973, 279 p. (in Russian)
3. Giovanetti A., Szetela I. Study of the gradual coking of the fuel piping system of turbojet engines at increased temperatures. Aerokosmicheskaya Technica. N7, 1987, pp. 95-102.
4. Altunin V.A. Study of Effect of the Electrostatic and Magnetic Fields on Features of Heat Transfer to Hydrocarbon Fuels and Coolants. Kazan State University, Kazan, 2006, 230 p. (in Russian)
5. Spalart, P. R. and Allmaras, S. R. "A One-Equation Turbulence Model for Aerodynamic Flows", AIAA Paper 92-0439, 1992.

6. CFD-ACE Modules Manual [Electronic Resource]. www.esi-cfd.com

7. Valiskóa M., Boda D. Correction to the Clausius–Mossotti equation: The dielectric constant of nonpolar fluids from Monte Carlo simulations. The Journal of Chemical Physics. V. 131, N16, 2009, pp. 120-123.

8. Kulikovsky A., Lyubimov G. Magnetohydrodynamics. Moscow, Logos, 2005, 328 p.

9. Dendy R.O. Plasma Dynamics. Clarendon Press, Oxford, 2002, 172 p.

10. A. Yoshigawa, S.I. Itoh, K. Itoh. Plasma and Fluid Turbulence: Theory and Modelling. CRC Press, 2002, 459 p.

11. Miakochin A.S., Yanovskiy L.S. Formation of Deposits in the Fuel Systems of the Power Units and Methods for Their Elimination. MAI, Moscow, 2001, 224 p. (in Russian)