Modelling of heating of plasma-chemical reactor in Comsol Multiphysics.

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Abstract. For the thermophysical calculation of the reactor, a mathematical model was developed in Comsol Multiphysics, describing physical processes in the plasma-chemical reactor at a stationary mode. To simplify the calculation at this stage, it was carried out for an air plasma torch. The model includes two processes: fluid dynamic and heat transfer ones. As a result of the mathematical modelling the following parameters were obtained: temperature distribution in the reactor at steady state, average mass temperature in the reaction volume, velocity field and others.

1. Introduction
At present, mathematical modeling has become an integral part of any research. It allows assessing correctness of the choice of a particular technical solution at the design stage. At the same time, mathematical modeling enables us to approach the final result with no physical models or prototypes [1,2]. Plasma technologies have been used in various industries for a long time. In recent years, the plasma technologies are becoming more and more popular since they aid to recycle waste [3,4] and plasma coating [5] more efficiently than traditional methods. The main processes of decomposition and destruction of waste by the plasma method take place in a plasma-chemical reactor. For example, to decompose organochlorine compounds it is necessary to keep it in a zone with a temperature of 1500 K for at least 2 seconds [6,7]. For this purpose, the reaction space is preheated with an air plasma torch for several hours. In the mathematical modeling of a plasma chemical reactor the uniformity of heating of the whole reaction space, the velocity field and the thermal losses of the reactor when bringing into the operation mode are of particular interest.

2. Model of plasma-chemical reactor
2.1. Assumptions and simplifications of calculation model
For the thermophysical calculation of the reactor, a mathematical model was developed, which describes the physical processes in a plasma-chemical reactor at a steady state. At this stage, the calculation was carried out for an air plasma torch. The model includes two physical processes: gas flow and heat transfer in gas and solids. In this work the model of the processes under consideration are simplified. Nevertheless, the results of modeling are scientifically and practically valuable.

The following simplifications are assumed:

- Plasma-forming medium is air.
- Chemical interaction between air components is lacking.
- Electric arc processes are excluded.
- Outflow from plasma torch is modeled by the flow rate, the power and the average working gas temperature [7,8].
- Radiation losses are not taken into account.

The aims of modeling the plasma-chemical reactor are:

- Design model of the existing plasma chemical reactor;
- Calculation of the velocity, temperature and pressure fields;
- Determination of the thermal losses power of the process, estimation of its share in the total energy input;

2.2. Geometry of computational domain

The scheme of the plasma-chemical reactor used in the Institute of Electrophysics and Electric Power of the Russian Academy of Sciences is presented in Fig.1.

![Fig. 1. Plasma-chemical reactor](image)

1 - reaction space; 2- refractory concrete Alkor-90; 3 - insulating concrete Alaks-1.6-1600; 4 – insulating board MKRP-340; 5- vessel of 12X18H10T steel.
2.3 Set of equations.
Model of the plasma-chemical reactor is described by equations of gas dynamics and heat transfer. The Navier-Stokes equation (1) describing motion of the compressible gas and the continuity equation are to be solved (4.2). Equation (4.3) describes heat transfer in the gas and reactor vessel.

\[
\rho \left( u \nabla \right) u = \nabla \cdot \left( -p I + \mu \left( \nabla u + \left( \nabla u \right)^T \right) - \frac{2}{3} \mu (\nabla \cdot u) I \right) + F
\]  
\[\nabla \cdot (\rho u) = 0 \]  
\[
\rho \cdot C_p \cdot u \cdot \nabla T + \nabla \left( -k \nabla T \right) = Q
\]

Here \( \rho \) is the gas density; \( u \) is the velocity field; \( p \) is the pressure; \( \mu \) is the viscosity; \( F \) are the external forces acting on the gas; \( C_p \) is the heat capacity; \( k \) is the thermal conductivity; \( q \) is the heat flow.

2.4 Initial and Boundary Conditions:
Initial pressure in the reaction volume is \( P = 101325 \) Pa. At the inlet to the reaction space, the velocity field at the exit from the plasma torch nozzles (Fig. 2) is set from the simulation model of the air ac plasma torch. Since it is difficult to simulate processes in AC plasma torches, the plasma flow is modeled by velocities and mean mass temperatures.

**Fig. 2.** Field of gas velocities at the exit from the plasma torch in the form of component expansion

Rarefication of 0.2 kPa is maintained at the outlet from the reaction space. Condition of non-percolation (the normal velocity component \( V_n = 0 \)) is set on the walls of the reaction space of the reactor. The influence of gravity is taken into account. At the inlet into the reaction space, the temperature distribution is determined (Figure 3), which is also obtained from the model of the three-phase ac plasma torch.
Temperatura field of the gas at the inlet into the reaction volume

The initial temperature of the entire design area is set $T = 293.15$ K. The convective heat flux (4) is specified from the boundaries of the design area.

$$q = h(T_{\text{ext}} - T); h = h_{\text{air}}(L; p_A; T_{\text{ext}})$$  \hspace{1cm} (4)

The main difficulty in using heat transfer coefficients is to calculate or determine the corresponding value of the coefficient $h$. This coefficient depends on the cooling flow, the properties of the flow material and the surface temperature and for forced convection cooling from the flow velocity. In addition, the coefficient is affected by the geometric configuration. The heat exchange interface provides built-in functions for heat transfer coefficients. For most technical purposes, applying these coefficients is an accurate and numerically efficient approach to modeling. Handbooks on heat transfer usually contain a large set of empirical and theoretical corrections for the coefficients $h$. The heat transfer module contains such a subset. These expressions are based on the following dimensionless quantities: $Nu$ (Nusselt number), $Re$ (Reynolds number), $Pr$ (Prandtl number), $Ra$ (Rayleigh number), $Gr$ (Grashof number).

In the model under consideration, heat transfer is given by external natural convection, where the geometric arrangement must be specified to calculate the heat transfer coefficient. For calculation, the following parameters are used: $h$ – heat transfer coefficient ($W/(m^2 \cdot K)$), $L$ – linear dimension (m), $\Delta T$ – The difference between surface temperatures and the volume of the cooling stream (K), $g$ – acceleration of gravity (m/s²), $k$ – flow thermal conductivity ($W/(m \cdot K)$), $\rho$ – flux density ($kg/m^3$), $U$ – volumetric flow rate (m/s), $\mu$ – dynamic viscosity ($Pa \cdot s$), $C_p$ – flow capacity ($J/(kg \cdot K)$), $\beta$ – thermal expansion coefficient (1/K).

Vertical wall:

$$h = \begin{cases} \frac{k}{L} \left(0.68 + \frac{0.67 k_{A}^{1/4}}{(1 + \frac{0.492 k_{A}}{\rho C_p})^{1/6}}T_{\text{ext}}\right), & Ra \leq 10^6 \\ \frac{k}{L} \left(0.825 + \frac{0.387 k_{A}^{1/6} \frac{g}{(1 + \frac{0.492 k_{A}}{\rho C_p})^{1/3}}}{}\right), & Ra > 10^9 \end{cases}$$  \hspace{1cm} (5)
The horizontal plate, the upper side of the reactor: If $T > T_{\text{ext}}$, then

$$
\begin{align*}
  h &= \begin{cases} 
    \frac{k}{l} 0.54 Ra^{0.25}, & Ra \leq 10^7 \\
    \frac{k}{l} 0.15 Ra^{0.33}, & Ra > 10^7
  \end{cases} 
\end{align*}
$$

(6)

While $T \leq T_{\text{ext}}$, then

$$
  h = \frac{k}{l} 0.27 Ra^{0.25} 
$$

(7)

$Ra$ is calculated in the same way as for a vertical wall. The horizontal plate, the lower side of the reactor. Equation (6) is used for $T \leq T_{\text{ext}}$, and equation (7) is used for $T > T_{\text{ext}}$. Otherwise it is also used as for a horizontal surface from the upper side. Geometric parameters are determined for the regions, for which the condition of convective heat transfer and ambient temperature $T_{\text{ext}} = 293.15$ K are set. The heat exchange interface provides built-in functions for the heat transfer coefficients. For the most technical purposes application of these coefficients is an accurate and numerically efficient approach to modeling.

2.5. Calculation method

Thermophysical calculation of the reactor is a stationary problem. For this purpose, a stationary solver was chosen where the solution was divided into sub-steps (segregated steps). This approach is called a separate solution. To solve a linear system of equations one can use an optimal solver for every process either direct, or iterative one, which is less resource-intensive. Each separate step may be a non-linear problem in itself, which may be solved with the desired error and controlled relaxation depending on a specific physical task. In the first step, we solve the equations for temperature, in the second for velocity and pressure. The total number of iterations was set to 300, the solution was achieved by Newton's method with damping coefficients of 0.5 in the first case and 0.8 in the second one. In each step the PARDISO solver was used.

3. Results

The calculation took 2 hours 50 minutes 20 seconds, it was carried out on a computer with AMD A10-7850K Radeon R7, 4 cores, 16 GB. The following parameters were obtained from the mathematical model:

1. Temperature distribution in the reactor at steady state is presented in Fig. 4. The average mass temperature in the reaction volume exceeds 1500 K.
2. Velocity fields are presented in Figs. 5-7. The data obtained indicate a turbulent flow regime in the reactor that promotes better mixing and improves completeness of transformation of the starting materials.
3. Estimation of the thermal losses power shows it makes up 9.3% (5.8 kW) of the plasma torch power (62.3 kW). Taking into account the radiative heat transfer, this value will be even greater.
4. Conclusion
The average mass temperature in the reaction volume exceeds 1500 K that meets the reaction conditions (decomposition of organochlorine compounds). Thermal losses are 9.3%. The high level of heat loss is due to the experimental type of the reactor and inherent in the small-capacity plants. When designing industrial installations, heat losses will be minimized by introducing additional technological chains for its useful utilization.

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