Calculation of Distribution Dynamics of Inhomogeneous Temperature Field in Range of Fuel Elements by Using FreeFem++

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Abstract. This article introduces the result of studying the heat exchange in the fuel element of the nuclear reactor fuel magazine. Fuel assemblies are completed as a bundle of cylindrical fuel elements located at the tops of a regular triangle. Uneven distribution of fuel rods in a nuclear reactor’s core forms the inhomogeneity of temperature fields. This article describes the developed method for heat exchange calculation with the account for impact of an inhomogeneous temperature field on the thermal-physical properties of materials and unsteady effects. The acquired calculation results are used for evaluating the tolerable temperature levels in protective case materials.

1. Introduction
The main purpose of the reactor thermal calculation is determination of temperature fields in its structural elements in normal, transition, and emergency mode.

One of key tasks of the reactor calculation is determination of temperature fields in fuel elements. Fuel elements operate in extremely tense conditions: high temperatures, heavy heat release, and high radiation level are often accompanied by chemically aggressive heat-bearing agents flowing around the surface of fuel elements. Along with that, fuel elements must meet severe requirements for their reliability, as fault of several fuel elements may lead to emergency situation. Reliability of a fuel elements significantly depends on proper selection of its temperature mode, as temperature strongly affects structural behavior of fissionable and structural materials, as well as intensity of radiation-chemical transformations running in fuel.

Distributions of temperature fields and heat flows in a nuclear reactor’s fuel element were studied by slew of authors, for instance, [1-3]. Analytical and numerical solutions of linear thermal conductivity equations were found. At high temperatures and heavy heat release rates, taking thermal-physical properties of materials as constant values will not be sufficient. In this regard, new methods for calculation of temperature fields must be developed and consider time- and space-specific changes in heat release properties.
Papers [4,5] introduce problems of heat exchange in a fuel element and suggest methods for calculation of temperatures in a fuel element with various elements and their thermal-physical properties and energy releases.

2. Math modeling

The article presents a problem of unsteady thermal conductivity with equally distributed internal heat source with inhomogeneous boundary conditions. The fuel assembly comprises no more than three elements. Materials’ thermal conductivity coefficients are determined by the given dependence on a temperature field. To date, fuel rods cases made of the zirconium alloy (Zircaloy 4) are essentially used. Along with zirconium itself, this alloy also contains tin, iron, and chrome.

The paper [6] presents the Zircaloy 4 thermal conductivity function depending on temperature as follows:

\[ \lambda(T) = 8.8527 + 7.082 \cdot 10^{-3} T + 2.5329 \cdot 10^{-6} T^2 + 2.9918 \cdot 10^{-4} T^{-1} \]  

(1)

For the purpose of describing heat exchange processes in the nuclear reactor’s channel, the homogeneous environment flow model is used. Beginning from \( t = 0 \), heat release rate starts changing exponentially [7]:

\[ q_i(t) = q_{i0} \cdot \exp(k \cdot t) \]  

(2)

Let us denote the cross-section of a fuel element consisting of a rod (fissionable material) and three protective case, by \( \Omega = \Omega_0 \cup \Omega_1 \cup \Omega_2 \cup \Omega_3 \), where

\[ \Omega_0 = \{(R, \varphi): 0 \leq R \leq R_0, 0 \leq \varphi \leq 2\pi\}; \]
\[ \Omega_1 = \{(R, \varphi): R_0 \leq R \leq R_1, 0 \leq \varphi \leq 2\pi\}; \]
\[ \Omega_2 = \{(R, \varphi): R_1 \leq R \leq R_2, 0 \leq \varphi \leq 2\pi\}; \]
\[ \Omega_3 = \{(R, \varphi): R_2 \leq R \leq R_3, 0 \leq \varphi \leq 2\pi\}. \]

(3)

where \( R_0 < R_1 \leq R_2 \leq R_3 \), \( R_0 \) is the non-dimensional radius of a fuel element’s rod, \( R_i, R_2, R_3 \) are non-dimensional radiiuses of a fuel element’s cases.

Differential equations for describing temperature fields in the fuel assemble are as follows [7]:

\[ \frac{\partial T_i}{\partial F_0} + \Delta T_i = -2 \cdot (R_i / R_0)^2 \cdot \exp(k \cdot m \cdot F_0), \quad (x,t) \in \Omega_i \times (0,t); \]  

(4)

\[ \frac{\rho_i \cdot c_{pl}}{\rho_0 \cdot c_{pl}} \cdot \frac{\partial T_i}{\partial F_0} + \frac{\lambda(T)}{\lambda_0} \cdot \Delta T_i = 0 \quad (x,t) \in \Omega_i \times (0,t), \quad i = 1,2,3. \]  

(5)

here, \( \Omega_i, i = 1,2,3 \) are areas determined in Ошибка! Источник ссылки не найден., where \( R_i = R_i / R_0, T_0, T_i, i = 1,2,3 \) are non-dimensional flow temperature fields of a rod and cases of a fuel element respectively, \( \rho_i, c_{pl}, i = 0,\ldots,3 \) are densities and heat capacity ratios of environments corresponding to (3), \( \lambda_0 = const \) is a rod’s thermal conductivity coefficient, \( \lambda(T) \) is the thermal conductivity function of a fuel element’s protective elements, determined in equation (1), \( m = R_3^2 / a_0, k = 0.03 \) is reactor life-time. The temperature scale is denoted by \( \Theta_q = q \cdot d / \lambda_2 \), which has the temperature dimension.

Let us write boundary and initial conditions. As \( R = 0 \) for a temperature field \( T_0 \), the impermeability condition is laid:
\[
\left(\frac{\partial T_0}{\partial R}\right)_{R=0} = 0.
\]

On the boundary between a rod and case, as well as between cases, the equality of temperatures and heat flow densities is assumed:

\[
T_i(R_i) = T_{i+1}(R_i),
\]

\[
\left[\lambda(T_i) \cdot \frac{\partial T_i}{\partial R}\right]_{R=R_i} = \left[\lambda(T_{i+1}) \cdot \frac{\partial T_{i+1}}{\partial R}\right]_{R=R_i},
\]

\[i = 1, 2, 3, \quad 0 \leq \varphi \leq 2\pi\]  

(7)

In case of considerably close spacing of fuel elements in the bundle, heat exchange coefficient turns out to be inconstant across the round of fuel rods, depending on angle \(\varphi\) \([7,8]\):

\[
T_3(R_3, \varphi) = T_f + \sum_{k=1}^{\infty} a_k \cdot \cos(6 \cdot k \cdot \varphi),
\]

where \(T_f\) is the average temperature of a fuel element’s surface. This paper assumes coefficients \(a_k\) as given.

As an initial condition, the distribution of a temperature field is taken, found from the steady-state problem corresponding to (4) – (8) Figure 1.

Numerical solution of an unsteady problem (4) – (8) was found by using the finite element method and applying the FreeFem++ integration. Analysis of convergence of the found solution at two calculation grids differing from each other in the number of points (2 times), revealed that solution convergence is reached at the number of grid points of about 1223.

Results of the numerical solution provide for determining the thermal conductivity coefficient \(\lambda(T)\). Figure 2 shows values of thermal conductivity design coefficients found at initial and final time, considering time-dependent distribution of a temperature field in cases.
Geometric parameters of a fuel unit are as follows:

\[ R_0 = 0.02 \text{ m}, R_1 = 0.0205 \text{ m}, R_2 = 0.021 \text{ m}, R_3 = 0.0215 \text{ m} \]

Average temperature is 380°C, capacity of internal heat sources in the fuel pellet is

\[ q_{i0} = 6.9 \cdot 10^7 \text{ [W / m}^3\text{]} \]

Unsteady-state equation of thermal conductivity, describing time-dependent change of temperature \( T(R; t) \), takes the following form [7, 8]:

\[ \frac{\partial T}{\partial t} - a(T) \cdot \Delta T = Q(t) \]  

where \( Q(t) \) is frequency distribution of internal heat sources, \( a(T) = \lambda(T)/(\rho \cdot c_p) \) is coefficient of thermal diffusivity.

Let us consider a case when Dirichlet conditions are laid on the outer boundary, which correspond to temperature \( T_c(R, t) \) on the boundary:

\[ T \big|_{R=R_3} = T_c(\varphi; t) \]  

The steady-state problem solution is taken as the initial temperature distribution:

\[ T(R; \varphi; 0) = T_s(R; \varphi) \]  

Time-dependent approximate derivative. We seek a problem solution falling within the time interval \([0, t_n]\). Let us set a range of values \( t_n = n \cdot \tau \) on this interval, where \( \tau \) is a time step. For function \( T \) at time \( t_n \), let us introduce the following notation:

\[ T_n(R; \varphi) = T(R; \varphi; t_n) \]  

Let us approximate the time-dependent derivative with the finite difference [9]:

\[ \frac{dT(R; \varphi; t)}{dt} \bigg|_{t=t_n} \approx \frac{T_{n+1}(R; \varphi) - T_n(R; \varphi)}{\tau} \]
During calculation, the thermal conductivity coefficient of a case is taken as temperature-dependent and calculated by (1) through using the iterational process. Considering (12) – (13), let us write the finite-difference equations for the problem (9) – (11):

\[
\frac{T_{n+1} - T_0}{\tau} - a(T_{n+1}) \cdot T_{n+1} = Q_{n+1},
\]

\[
T_{n+1}(R; \phi; t) = T_c(\phi; t),
\]

\[
T_0 = T_s(R; \phi).
\] (14)

Let us write the weak statement of the problem (14) by using the partial integration formula [10]. The problem (14) is nonlinear, and must be solved iteratively. If \( n \) denotes the iteration index, a semi-linearization of the non-linear condition gives

\[
(T_{n+1}, H) + \tau \cdot (a(T_n) \cdot \nabla T_{n+1}, \nabla H) = (T_n, H) + \tau \cdot (Q_{n+1}, H),
\]

\[
a_{n+1/2} = \left( \frac{\lambda_{n+1/2}}{\lambda_{n+1/2}} \right) \left( \rho \cdot c_p \right),
\]

\[
\lambda_{n+1} = \left[ 8.8527 + 7.082 \cdot 10^3 \cdot T_{n+1} + 2.5329 \cdot 10^5 \cdot (T_{n+1}, H)^2 + 2.9918 \cdot 10^5 \cdot (T_{n+1})^{-1} \right],
\]

\[
(T_{n+1}, H) + \tau (a_{n+1/2} \cdot \nabla T_{n+1}, H) = (T_n, H) + \tau (Q_{n+1}, H), \quad n = 0, \ldots, N,
\]

\[
T_{n+1}(R; \phi; t) = T_c(\phi; t),
\]

\[
T_0 = T_s(R; \phi).
\] (18)

The suggested scheme (15)-(18) for determining a temperature field in the bounded area is used to find a solution to the problem (4) – (8) within \( \Omega = \Omega_0 \cup \Omega_1 \cup \Omega_2 \cup \Omega_3 \), where \( \Omega_0, \Omega_1, \Omega_2, \Omega_3 \) are determined in (3).

The graph of a solution to the unsteady-state problem (4) – (8) is given in Figure 3.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{Graph of an Unsteady-State Problem Solution.}
\end{figure}

Initial temperatures \( T_0(R, \phi) \) in Figure 3 correspond to the steady temperature distribution in a fuel unit (Figure 1). The calculation was made within a 60-sec time range. Figure 3 displays the fuel reaches the melting point in the fuel element center in 60 seconds.
3. Conclusion

The numerical calculation achieved enables to conduct evaluation of temperature distribution throughout the cross-section of a fuel element at any given time, as well as to evaluate the thermal conductivity coefficient depending on capacity of fuel pellet heat sources, temperature of a heat-bearing agent and external heat sources. This method provides for determining the time-dependent change of the thermal conductivity coefficient in protective elements of a fuel element. The dynamics of changes of protective elements’ thermal conductivity coefficient is given in Figure 4.

![Graph of Time-Dependent Change of Thermal Conductivity Coefficient.](image1)

The change of steady and unsteady temperature fields in protective cases is given in Figure 5.

![Graph of Temperature Change in a Fuel Element’s Protective Elements.](image2)

Figure 6 presents the dynamics of change of temperature fields in the center and on the boundary of a fuel element's pellet.

This calculation enables to consider the number of protective elements, their thermal-physical properties, impact of adjacent fuel elements belonging to a nuclear reactor’s core.

![Graph of Time-Dependent Temperature Change.](image3)
The dynamics of temperature fields distribution is affected by the capacity of internal sources and irregularity of a heat-bearing agent’s temperature.

Numerical modeling of a heat release process provides for selecting the internal sources’ capacity that ensures the optimal operation mode of a nuclear reactor.

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