Calculation of the problem of thermoplasticity on the example of a stationary power plant flange using free software Code_Aster

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Abstract. The construction of a geometric model and finite element approximation of the flange of a stationary power plant is presented. Modelling and meshing were held using Salome-Meca modules. The paper provides a brief description of the key commands in AsterStudy module for modeling this problem. A numerical calculation of the heat-stress state of the flange of a stationary power plant was performed using free Code_Aster software. Distributions of temperature for four periods, flange deformation, displacements, and also equivalent von Mises stresses are given as a results of the study.

1. Introduction
An important stage in the design of installations in industries is the calculation of temperature and stress fields in structural elements, operating at high temperatures. At the same time, temperature and stress field remains at a constant, but sufficiently high level even in stationary modes, which leads to the accumulation of damage [1, 2].

The finite element method (FEM) is widely used to calculate the heat stress state of structural elements. One of the options for calculating machine components is the use of libraries of finite element programs, written in compiled high-level programming languages.

An alternative to the previous approach is to use software finite element complexes. A large number of both commercial software finite element complexes, such as ANSYS, Abaqus, MSC.Nastran, LS-Dyna, and free software (Code_Aster, CalculiX, Elmer, etc.) exist. It is relevant to use free software for calculating the heat-stressed state of structural elements due to independence from owners of commercial licenses. Moreover, it eliminates high cost of software and widen possibilities for adapting the code for solving specific problems. However, the choice of a free software package requires validation test calculations [4].

The paper presents a solution of the non-stationary thermoplasticity problem for flange of a stationary power plant. The calculations were carried out using free software package Code_Aster.

2. Functional content of the Salome-Meca package
SALOME, being open source software, provides a common pre- and post-processing platform for numerical simulation. The package can be used as an application for creating a CAD model,
preparing it for numerical calculations, including the construction of two-dimensional and three-dimensional meshes, and the subsequent processing of the calculation results.

Salome-Meca is a standalone application that integrates the Code_Aster solver into the SALOME platform. The main modules of this package are: the Geometry and Mesh modules inherited from SALOME, the AsterStudy module, which represents the Code_Aster solver, and the ParaVis module for visualizing the results obtained during the solution process. A feature of the package is the ability to access all functions through the integrated Python console.

The Geometry module allows you to create geometric objects of varying complexity using the provided set of tools. Geometry provides the ability to import and export generated geometric models. The Mesh module provides several ways to create a mesh: building from a geometric object, importing and exporting in various formats, combining several meshes, or copying a part of a mesh to a new one.

Code_Aster (acronym for Analysis of Structures and Thermomechanics for Studies and Research) is a free software package for solving problems of mechanics, hydromechanics, thermal conductivity, acoustics, related thermomechanics problems, and problems generated by vibration processes, by the finite element method. The solver has all the necessary set of commands for solving nonlinear problems, it offers advanced functionality for fatigue analysis of structures, fracture mechanics and seismic analysis.

ParaVis is a module representing a cross-platform ParaView data visualization application. Ease of use, flexible and intuitive user interface allows to quickly and clearly present the results for further analysis.

3. Mathematical model

The formulation of the associated stationary thermomechanical problem in the region \( V \), corresponding to a homogeneous body of isotropic material has the form [2]:

\[
\Delta T(M) = 0, \quad \nabla \cdot \sigma(M) = 0, \quad M \in V, \quad (1)
\]

\[
\sigma = \frac{E}{1 + \nu} \left( \dot{\varepsilon} + \frac{\nu}{1 - 2\nu} \varepsilon \hat{I} - \alpha^{(T)} (T(M) - T_0) \hat{I} \right), \quad (2)
\]

\[
\dot{\varepsilon} = \left( \nabla u + (\nabla u)^T \right) / 2, \quad (3)
\]

where \( \Delta \) is the Laplace operator; \( T(M) \) is the temperature, [K]; \( \sigma \) is the stress tensor, [Pa]; \( E \) is the Young’s modulus, [Pa]; \( \nu \) is the Poisson’s ratio; \( \varepsilon = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} \); \( \hat{I} \) is a unit tensor of the second rank; \( \nabla \) is the Hamilton operator; \( \alpha^{(T)} \) is a coefficient of thermal deformation, [K\(^{-1}\)]; \( u \) is a displacement vector.

The boundary conditions for such a problem have the form:

\[
T|_{S_1} = f_1(x), \quad q|_{S_2} = f_2(x), \quad \sigma|_{S_3} = p(x), \quad u|_{S_4} = g(x), \quad (4)
\]

where \( S_1 \cup S_2 = \partial V, \ S_3 \cup S_4 = \partial V, \ S_1 \cap S_2 = \emptyset, \ S_3 \cap S_4 = \emptyset \), \( q \) is a heat flux density vector; \( \sigma \) is a stress vector; \( f_1(x), f_2(x), p(x), g(x) \) are known function and vector functions.

The flange of a stationary power plant, made of high alloy steel, is considered. Typical flange dimensions in millimeters are shown in figure 1.
By placing the origin of the coordinate system at the center of the flange, the solid model is split into four parts by planes of symmetry, perpendicular to the coordinate axes $Ox$ and $Oy$. The fragment located in the first octant is taken for further consideration (figure 2).

The initial temperature of the flange is 283 K. Sections (6), (7) belonging to the planes of symmetry of the geometric model, as well as sections of surfaces (4) and (5), perpendicular to the $Oz$ axis, which are zones of contact with adjacent structural elements, and finally, cylindrical surfaces of holes for fasteners are considered to be thermally insulated. The inner surfaces (1) and (2) of the flange are in contact with the medium. Figure 3 shows the dependence of the temperature of the medium $T_c$ on time, which is a periodic change with a period of 720 s. Plots of the heat transfer coefficients $\alpha_1$ and $\alpha_2$ of surfaces (1) and (2) versus time are also periodic (figure 4).

![Figure 1. Flange dimensions in millimeters.](image1)

![Figure 2. Fragment of a solid model of a stationary power plant flange.](image2)

![Figure 3. Temperature of the medium versus time graph.](image3)
Figure 4. Graphs of the dependence of the heat transfer coefficients $\alpha_1$ and $\alpha_2$ on time.

On the outer surface (3) of the flange heat exchange occurs with an environment of constant temperature $T_3 = 283$ K, the heat transfer coefficient is $\alpha_3 = 15$ W/(m·K). Apart from the thermal effect, the inner surfaces (1) and (2) of the flange are subject to mechanical stress — pressure $p = 7.5$ MPa, which arises with a period of 12 minutes and acts during the first half of each period. At the initial moment of time $t = 0$, the loading is assumed to be instantaneous.

4. Building a solid model and finite element approximation

A solid model of a flange fragment was built in the Geometry module of the Salome-Meca package using a standard set of built-in commands. To simplify the further construction of the finite element approximation, planes that split the flange fragment into parts were additionally built. Surfaces, on which the boundary conditions will be imposed, were selected from the 3D model for the correct operation of the mesh algorithms [10].

A mesh (figure 5), the elements of which are first-order tetrahedra [3], was automatically generated, using Mesh module. The range of lengths of the edges of the tetrahedra and surfaces to which the mesh is to be thickened, are indicated. Groups of elements, based on the geometric model are selected from the mesh for further definition of the boundary conditions. The mesh contains 3035 nodes and 9142 tetrahedron.

Figure 5. Mesh with elements in the form of tetrahedrons.
5. Determination of material and boundary conditions for solving a nonlinear heat conduction problem

Steel 321S51 was taken as the material from which the flange was made. Density of steel is $\rho = 7800 \text{ kg/m}^3$ and specific heat value $c = 650 \text{ J/(kg·K)}$. The temperature dependence of the thermal conductivity coefficient $\lambda$ is shown in figure 6.

![Graph of the dependence of the thermal conductivity coefficient $\lambda$ on temperature.](image)

Figure 6. The graph of the dependence of the thermal conductivity coefficient $\lambda$ on temperature.

The standard algorithm of modelisation to follow in the AsterStudy module involves step-by-step modeling of the task in accordance with the sequence of commands set in the package, fixed on the toolbar above the workspace. At the first stage, which is solving the problem of thermal conductivity, the constructed mesh is read, the type of modeling is determined: MODELIZATION > 3D, and the main characteristics of the material are set. The thermal conductivity coefficient, as well as the medium temperature $T_c$ and the heat transfer coefficients $\alpha_1$ and $\alpha_2$ are set in a tabular way. Constants such as heat flow, volumetric heat capacity, temperature $T_3$ and heat transfer coefficient $\alpha_3$ are defined as constant functions. Since the part of the flange is made of a homogeneous material, these specifications apply everywhere.

6. Consideration of the boundary conditions in the process of modeling the heat conduction problem

Boundary conditions are associated with the groups of elements selected at the stage of mesh creation. Since most parameters are not constant values, the AFFE_CHAR_THER_F command is used to take into account the boundary conditions.

The purpose of creating a list of time steps and choosing the optimal step for nonlinear calculation is to achieve a compromise between desires, on the one hand, to make the step large enough to reduce the calculation time, and on the other hand, small enough to ensure that the solution converges at each time step. The AsterStudy solver module allows to automatically split the time step in the absence of convergence. This procedure can be performed according to a user-defined algorithm.

The DEFI_LIST_REEL command creates a list of real numbers equal to desired time steps, which is specified as the main one. Further, in case of absence of convergence, with the DEFI_LIST_INST command the time step is split into 5 parts by SUBD_PAS, if there is still no convergence, the time step can be again divided into 4 parts by SUBD_NIVEAU.

Creating a list listARCH = DEFI_LIST_REEL allows user to adjust the time step for writing the data obtained during the solution process to the output file of the results.
The solution to the nonlinear problem of thermal conductivity is determined by the THER NON LINE command, where, in addition to the load CHARGE = load, the initial flange temperature VALE = 283.0 and the list of time steps LIST_INST = listTime are specified.

7. Visualization of the results of solving a nonlinear heat conduction problem
Figure 7 shows the temperature distribution over the flange surface at the time \( t = 360 \) s. In figure 8 the numbers indicate the characteristic nodes for which the graphs of the temperature versus time are plotted.

Figure 7. Temperature distribution at time \( t = 360 \) s.

Figure 8. Characteristic nodes.

Figure 9 for nodes 6, 21, 373, 632 shows the temperature versus time graphs, according to which the temperature stops increasing by the fourth period.

Figure 9. Temperature graphs for nodes 6, 21, 373, 632 for 4 periods.
8. Definition of mechanical properties of material and boundary conditions
The mechanical properties of the steel 321S51 are determined by the following parameters: 

\[ \alpha(T) = 1.2 \cdot 10^{-5} \text{ K}^{-1}, \quad \nu = 0.3. \]

The strain diagram is a curve obtained by performing monotonic uniaxial tensile tests on a test piece. For this material a mathematical model of an elastoplastic continuous medium with linear hardening is adopted. The yield strength of steel is \( \sigma = 300 \text{ MPa} \), and the hardening factor is \( E = 250 \text{ MPa} \). The strain diagram is a curve obtained by performing a monotonic uniaxial tensile test on a test piece (figures 10, 11).

![Figure 10. Temperature dependence of Young’s modulus of steel.](image1)

![Figure 11. Tension diagram for steel (321S51).](image2)

9. Boundary conditions and solving the problem of thermoplasticity
Boundary conditions are taken into account by two commands: \texttt{AFFE_CHAR_MECA} is for fixing degrees of freedom of symmetry planes and cylindrical holes for fasteners, and \texttt{AFFE_CHAR_MECA_F} is for determining variable pressure \( p \). At the second stage, a nonlinear calculation of thermoplasticity is performed by the command \texttt{STAT_NON_LINE}.

COMPORTEMENT is short for comportement incremental, which can be translated as incremental behavior. The AsterStudy module saves the history of material behavior at each time step and, in the case of calculating the plasticity, based on the results from the previous step, according to the tension diagram, determines whether the material has reached the plastic deformation zone [7].

The loading process is accompanied by an increase in plastic deformations. The increments of deformations can be represented as the sum of increments of elastic and plastic deformations [5, 6]: 

\[ d\varepsilon_{ij} = d\varepsilon_{ij}^e + d\varepsilon_{ij}^p, \]

where \( d\varepsilon_{ij}^e \) is an increment of elastic deformations and \( d\varepsilon_{ij}^p \) is an increment of plastic deformations. Associated flow rule is 

\[ d\varepsilon_{ij}^p = d\lambda \frac{\partial f}{\partial \sigma_{ij}}, \]

where \( d\lambda \) is the Lagrange multiplier and \( f(\sigma_{ij}) \) is plastic potential.

The hardening type is specified by the \texttt{RELATION>VMIS_ISOT_LINE} keyword, i.e. isotropic hardening and material behavior is determined according to the tension diagram [8].
Code_Aster provides a wide range of models for describing material deformations, this problem uses a type that allows small (no more than 5%) displacements and plastic deformations. Thus the appropriate keyword is DEFORMATION = 'PETIT' [9]. The CONVERGENCE parameter defines the calculation error and the number of iterations for each time step. The value of the error is $10^{-4}$ and considered acceptable for the given problem, higher accuracy entails a significant increase in calculation time.

10. Visualization of the results of solving the problem of thermoplasticity
Figure 12 shows the deformation of the flange relative to the initial state. For clarity, the scale of displacements of mesh nodes was increased by 3 times. Figure 13 shows the numbers of mesh nodes for which graphs will be built further.

![Figure 12. Flange deformation (t = 360 c).](image)

![Figure 13. Characteristic nodes for graphing obtained data.](image)

Figure 12. Flange deformation (t = 360 c).

Figure 14 shows displacements along the axis Oz for two moments of time: $t = 360$ s, corresponding to the end of the first loading half-cycle and $t = 720$ s, corresponding to the end of the first unloading half-cycle.

![Figure 14. Displacements along the Oz axis at times t = 360 s and t = 720 s.](image)

Figure 14. Displacements along the Oz axis at times $t = 360$ s and $t = 720$ s.

According to the results obtained, the greatest load falls on the central zone of the flange adjacent to the cylindrical pipe. Figure 15 shows a graph of the time dependence of displacement along the Oz axis for two nodes 8494 and 10284.
Figures 16-17 show von Mises stresses and strains for two points in time, namely $t = 360$ s and $t = 720$ s. For better visual perception, the range of obtained values has been divided into 22 segments.
11. Conclusion
The work considered flange of a stationary power plant under thermal and mechanical loadings. Its solid geometric model and finite element approximation was built in modules imbedded in an open-source software Salome-Meca. Using free software Code-Aster and included solver module, the simulation and solution of the nonlinear problem of heat conduction, as well as the problem of thermoplasticity, were performed. In the text of this work emphasis was placed on the use of a number of key parameters during the modeling process, which allows for a correct calculation. The ParaVis module provides a graphical interpretation of the calculation results. Distributions of temperature for characteristic nodes for four periods, flange deformation, displacements, and also equivalent von Mises stresses was given. A conclusion was made about the part of the flange most exposed to loads, based on the results obtained.

Acknowledgements
The research was supported by the Ministry of Science and Higher Education of the Russian Federation, project No. 0705-2020-0047.

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