

# A code for 3D calculations of the output characteristics for a single-cell thermionic fuel element of thermionic nuclear power plants for different applications

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Available online 23 August 2017

## Abstract

R&D has been conducted by a cooperation of Rosatom State Corporation’s enterprises to build a line of autonomous small nuclear power plants (SNPP) of up to  $1\text{MW}_{\text{el}}$  to support government programs for the development of Russia’s Arctic region. In terms of heat and electricity supplies in an installed electric power range of 10 to  $100\text{kW}_{\text{el}}$ , the most attractive solution is offered by highly autonomous, compact and easy-to-maintain SNPPs with an in-core thermionic system. The key component of a thermionic NPP is a thermionic fuel element (TFE), which structurally integrates fuel and electrogenerating elements. Experimental studies and tests of thermionic plants are complex and expensive, so emphasis in the design of TNPPs is placed on mathematical simulation of physical processes taking place in the TFE. The paper considers the results of a 3D numerical simulation for the thermal and electrical characteristics of a single-cell TFE for a TNPP as part of one of the feasible SNPP designs, based on the procedure developed using COMSOL Multiphysics, an advanced software platform, and called by the authors COMSOL-EGK-SC. Initial data have been formulated to calculate a single-cell TFE, stages are described for the TFE mathematical model development in the COMSOL-EGK-SC software environment, and numerical calculation results for the thermal and electrical performance based on experimental data on the current–voltage characteristics (CVC) of a thermionic converter (TC) and the results of a neutronic calculation for the possible structure of the TNPP core as part of an SNPP are presented.

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**Keywords:** Thermionic NPP; Single-cell thermionic fuel element; Finite element analysis; 3D numerical simulation.

## Introduction

Conversion of thermal energy to the electric energy released in the nuclear fuel fission reaction is considered one of the most efficient ways to solve a range of long-term ground and outer-space tasks concerned with sustained electricity supplies to consumers at a level of dozens or more kilowatts [1–3]. To support government programs for the development of the Russian Federation’s Arctic region [4,5], R&D has been conducted by a cooperation of Rosatom State

Corporation’s enterprises to build a line of autonomous small nuclear power plants (SNPP) with a capacity of up to  $1\text{MW}_{\text{el}}$  satisfying to radiological, environmental and nuclear safety requirements [6]. The most attractive solution, in terms of heat and electricity supplies in an installed electric power range of 10 to  $100\text{kW}_{\text{el}}$ , is offered by highly autonomous, compact and easy-to-operate direct energy conversion SNPPs with an in-core thermionic system [7,8], which have confirmed their reference status by outer-space operations (Topaz nuclear propulsion system) and by ground tests (Yenisey nuclear propulsion system) [9,10].

At the present time, a project is being developed by a cooperation of Rosatom’s enterprises to build a thermionic nuclear power plant (TNPP) for SNPPs intended for electricity and heat supply to installations in Russia’s difficult-of-access and remote northland areas in conditions of no centralized power supplies and communication routes [6–8].

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Peer-review under responsibility of National Research Nuclear University MEPhI (Moscow Engineering Physics Institute).

Russian text published: Izvestiya vuzov. Yadernaya Energetika (ISSN 0204-3327), 2017, n.2, pp. 81–92.

<http://dx.doi.org/10.1016/j.nucet.2017.08.004>

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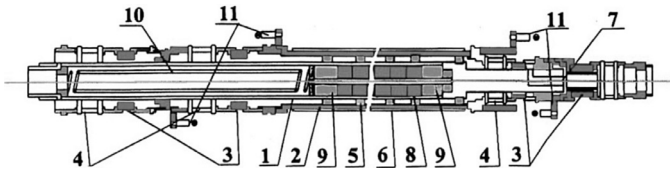


Fig. 1. Structural diagram of a single-cell SNPP TNPP TFE [8]: 1 – emitter; 2 – collector; 3 – sealed leads-in; 4 – bellows; 5 – spacers; 6 – electrical insulation; 7 – electrode gap; 8 – nuclear fuel; 9 – end reflectors; 10 – retainer; 11 – terminals.

The concept of the TNPP is based on the current technological advance, up-to-date designs, cutting-edge scientific achievements and hi-tech solutions. The key component of the TNPP is a thermionic fuel element (TFE) which structurally integrates electrogenerating and fuel elements. At large, the input and output characteristics of these devices are what the performance of the TNPP type under consideration depends on to a great extent. A single-cell TFE (Fig. 1) developed for the Yenisey nuclear propulsion system, which offers the best capabilities in terms of ensuring a long (reactor) life without degradation of the output characteristics, is considered as the potential choice for the base SNPP TNPP TFE [8,11].

### Problem statement

There are different coupled physical (neutronic, emission, plasma, adsorbing, thermoelectric, thermal-hydraulic, thermo-mechanical and other) processes taking place in a TNPP TFE. Experimental studies on and tests of thermionic plants are complex and expensive, so emphasis in the TNPP design is placed on mathematical modeling.

Such modeling makes it possible to predict the TFE output electric power and determine the TFE's internal parameters which cannot be measured directly in tests due to the specific design of a full-scale TFE (amount of heat released in a fuel element, distribution of the electrode temperature and potentials, etc.). Therefore, numerical simulation of the physical processes in single- and multi-cell TFEs, based on up-to-date 3D mathematical models, is a timely and practically important task.

The paper considers the results of a 3D numerical simulation for the thermal and electrical performance of a single-cell TFE as part of a feasible SNPP design, based on a procedure developed using COMSOL Multiphysics, an advanced software platform [12,13]. Called by the authors COMSOL-EGK-SC, this is a modification of an earlier procedure, COMSOL-EGK, developed by IPPE to calculate the performance of multi-cell TFEs. Input data have been formulated for the calculation of a single-cell (SC) TFE, stages are described for the TFE mathematical model development in the COMSOL-EGK-SC software environment [14], and numerical calculation results for the thermal and electrical performance based on experimental data on the TC CVC and the results of a neutronic calculation for the possible structure of the TNPP core as part of an SNPP are presented.

### Comsol-EGK-SC

The existing procedures to calculate the TFE characteristics include a number of peculiarities and assumptions which frequently reduce to a great extent the accuracy of the calculation results. Primarily, this is explained by the fact that the majority of the mathematical models used in these procedures are one-dimensional. Another peculiarity is that all of them are narrow-oriented (used to calculate a particular TFE design) and do not enable high-quality calculation of a more geometrically complex TFE. So, an improved TFE calculation procedure is expected to ensure the transition from one-dimensional to 3D numerical calculation of the TFE characteristics, to take into account in detail the effects the properties of structural materials and fluids have on the thermal and electrical processes in the TFE, and to make it possible to calculate TFEs in a geometry other than the geometry of generation I TFEs (Topaz and Yenisey).

COMSOL Multiphysics is the code for finite element calculations on complex scientific and technical problems. The solution of any problem is based on numerically solved equations in partial derivatives by finite element method in one-, two- or three-dimensional measurements. Based on the COMSOL Multiphysics code, a procedure for the 3D calculation of the TFE thermal and electrical performance, called COMSOL-EGK, was developed by the authors at IPPE in 2012 [13,15,16]. It should be noted that COMSOL-EGK was developed to model multi-cell TFEs but was found to be unfit, in its original form, for calculating the characteristics of single-cell TFEs as part of an SNPP TNPP. So, calculation of a single-cell TFE required a modification of COMSOL-EGK which has resulted in a new code called COMSOL-EGK-SC.

### Mathematical modeling of a single-cell TFE in the COMSOL-EGK-SC environment

#### *TFE geometrical calculation model*

The device under consideration has a complex structure consisting of diverse and interlinked components. The TFE calculation model, developed using geometrical modeling tools in the COMSOL-EGK-SC environment, is shown in Fig. 2. This model of a single-cell TFE has been developed in a 3D geometry. The figure presents a vertical cross-sectional view of the developed TFE model.

The peculiarities of a single-cell TFE lead to a high spatial non-uniformity of the heat fluxes and temperatures in its structural components.

#### *Mathematical model of a single-cell TFE*

The mathematical model of electrostatic processes in multi-cell TFEs, as it is implemented in the COMSOL-EGK code, [13,15,16] is based on a number of significant assumptions which do not make it possible to analyze the electrostatics in single-cell TFEs because of the electric current flowing differently in the TFE structural components, in other words,

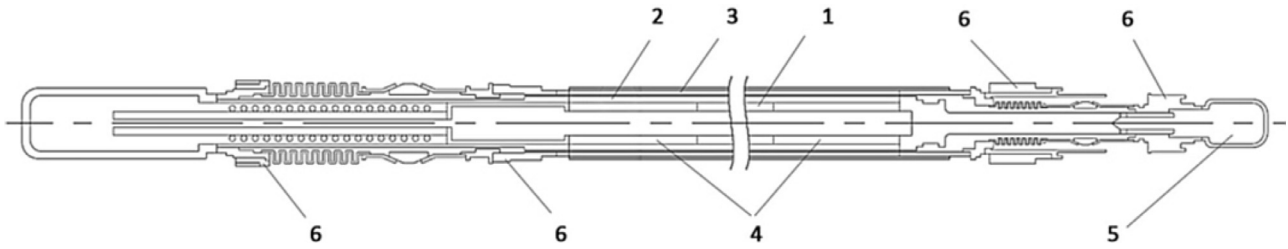


Fig. 2. A vertical cross-sectional view of a single-cell TFE: 1 – nuclear fuel, 2 – emitter, 3 – collector, 4 – end reflectors, 5 – fluid vapor generator (FVG), 6 – end components (terminals).

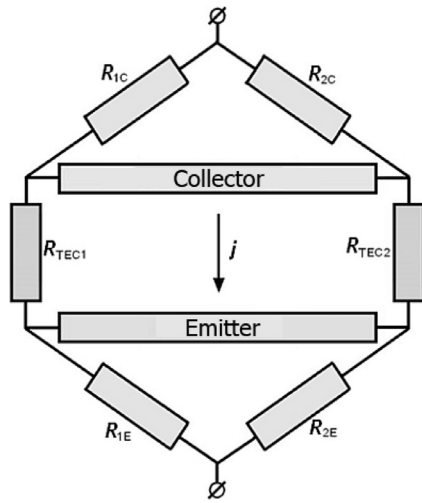


Fig. 3. Electrical circuit of a single-cell TFE.

because it has a differently shaped electrical circuit. Essentially, a single-cell TFE is a four-terminal network, including four connection points, two of which are inputs (leads-in) and the two other are outputs (terminals). It is important to note that the output electrical characteristics of a TFE depend to a great extent on the design and the electrical and thermophysical properties of its end component materials. This makes it impossible to use simplified one-dimensional models to calculate output electrical and thermophysical properties of the TFE without a major loss in accuracy. So, a peculiarity of the developed COMSOL-EGK-SC code is a modification of the TFE mathematical model enabling simulation of electrostatics and heat exchange in a four-terminal network with taking into account the irregularities caused by the complex geometry and the material composition of the single-cell TFE terminals. The electrical circuit of a single-cell TFE, as implemented in the COMSOL-EGK-SC code, is shown in Fig. 3.

#### Computational grid and material composition of the TFE model

The model of a single-cell TFE was split into finite difference elements using the COMSOL-EGK-SC code in a semi-automatic (adaptive) mode with the manual selection of the splitting type, as well as of the minimum and the maximum

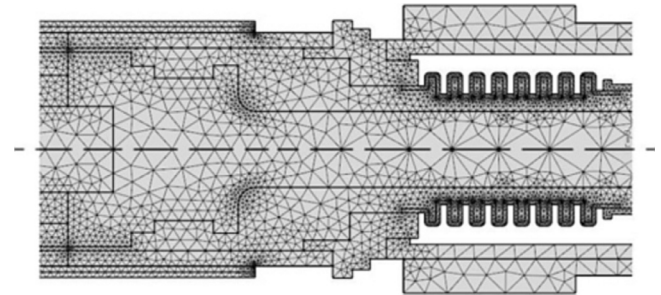


Fig. 4. A fragment of the TFE computational grid.

sizes of generated cells. As the result of the splitting used, the computational TFE model numbers more than 300,000 computational cells. A computational grid fragment is shown in Fig. 4.

The material composition of the TFE active part's structural components is presented in details in [8]. It is important to note that the COMSOL-EGK-SC code includes a built-in library of the physical properties of materials which was used for the subsequent calculation of the TFE electrical and thermophysical performance.

#### Closing relations of the TFE electrical and thermophysical calculation problem

The boundary conditions, which, essentially, are the closing relations in the TFE output characteristics calculation problem, include:

- distribution of the energy release from the TFE fuel column obtained as the result of a neutronic calculation for a core of the possible SNPP TNPP design and transferred in the form of tabulated data into the COMSOL-EGK-SC code (Fig. 5);
- an array of processed experimental data of the TC CVC corresponding to the TC mode of operation with the electrode pairs  $W_{\text{mono}}-\text{Mo}$  and  $\text{Pt-VKh2U}$  [17–19], for specifying the densities of the electrical current from the emitter surface and for coupling the TFE thermal and electrical calculation problems;
- distribution of the heat flux on the TFE can tube outer surface defined by the flow process and by the coolant properties, and specified in COMSOL-EGK-SC based on estimated thermohydraulic calculations for the SNPP TNPP.

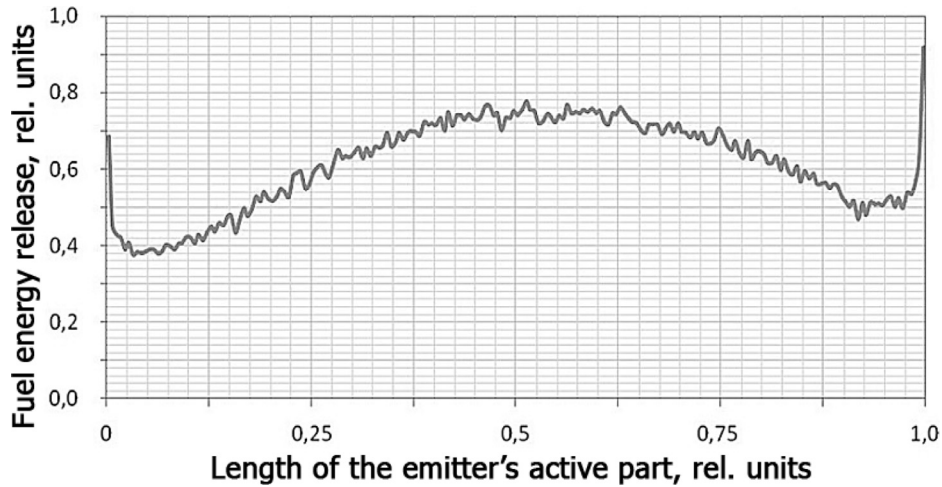


Fig. 5. Distribution of the TFE fuel composition energy release.

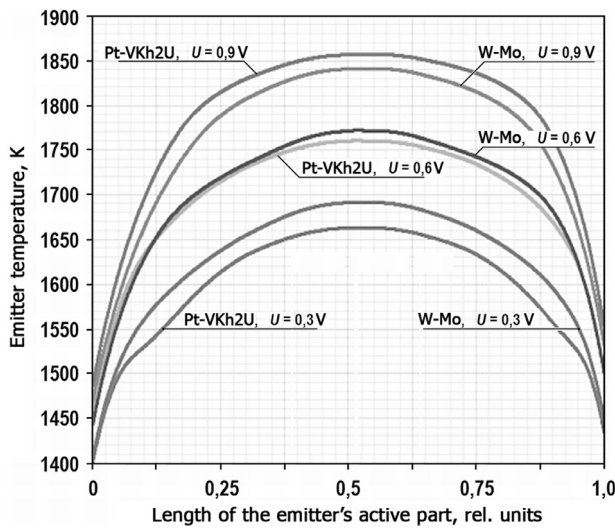


Fig. 6. Distribution of the emitter temperature along the TFE length for two types of the electrode pair materials at different electric voltage values.

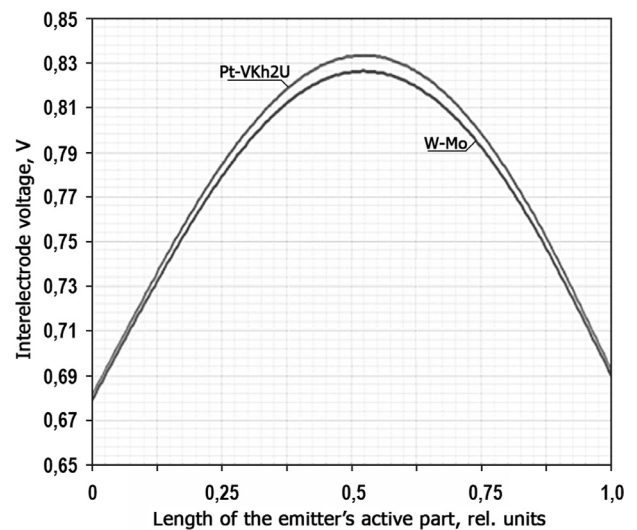


Fig. 7. Distribution of the interelectrode voltage along the TFE length for two types of the electrode pair materials at an electric voltage of 0.6 V.

**TFE performance numerical calculation results**

The key result of the TFE electrical and thermophysical performance calculations using the COMSOL-EGK-SC code are 2D temperature and electrical potential distributions for emitters, collectors and other structural components of the TFE. The distributions found are used to calculate the TFE CVC and the dependences of the electric power and the system efficiency on the electrical current flowing through the TFE [20]. As noted earlier, two samples of the experimental TC CVC for different materials of the electrode pair ( $W_{mono}-Mo$  and Pt-VKh2U) were used for the numerical calculation of the TFE characteristics. The calculations were performed for different thermal power values. Figs. 6–8 present calculated characteristics of a single-cell TFE as part of the SNPP TNPP obtained using the modified COMSOL-EGK-SC code.

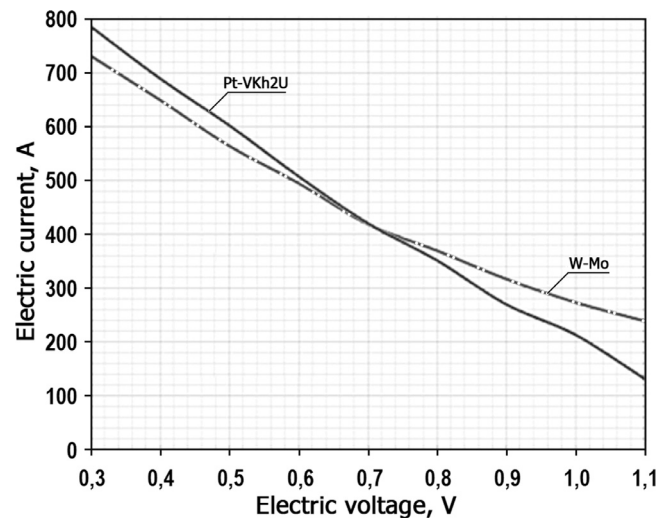


Fig. 8. Current–voltage characteristic of the TFE for two types of the electrode pair materials.

The obtained calculation results confirm a great deal of influence the spatial effects, which cannot be taken into account with the sufficient accuracy when one-dimensional mathematical models are used, have on the TFE's output electrical characteristics.

## Conclusion

A code, COMSOL-EGK-SC, has been developed as a modification of the COMSOL-EGK code for the computational justification of the characteristics of a single-cell TFE as part of a TNPP for different applications. In this code

- a detailed 3D geometrical model has been developed for a single-cell TFE as part of the SNPP TNPP;
- a mathematical model has been modified which makes it possible to simulate the electrostatics and heat exchange in a four-terminal network with regard for the irregularities caused by the complex geometry and the material composition of the single-cell TFE's terminals;
- two experimental databases on the CVC of a TC with the electrode pairs  $W_{\text{mono}}-\text{Mo}$  and  $\text{Pt-VKh2U}$  were used to calculate the TFE characteristics;
- distribution of the energy release from the single-cell TFE's fuel column was used, obtained as the result of a neutronic calculation for a version of the possible SNPP TNPP core structure.

High calculation accuracy has been achieved fully thanks to taking into account the real structure and the physical properties of the materials used in the modeled devices, as well as through the use of experimental data from the TC CVC database, the distribution of the TFE fuel composition energy release and the distribution of the heat flux on the TFE can tube outer surface which are the closing relations in the TFE output characteristics calculation problem. The use of the COMSOL-EGK-SC code to calculate the electrical and thermophysical characteristics of a single-cell TFE using a 3D mathematical model has shown the effectiveness and flexibility of the developed procedure.

The example provided in the paper on the application of the developed COMSOL-EGK-SC code does not limit its use only to justification of the single-cell TFE performance. It can be applied also to other TFE types (different material compositions, geometrical structures, boundary conditions, etc.) both with nuclear and nonnuclear heating.

The obtained results are a part of the R&D conducted under a government contract with Rosatom State Corporation by a cooperation of JSC Krasnaya Zvezda, SIA Luch and IPPE.

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