

Министерство науки и высшего образования Российской Федерации  
 федеральное государственное автономное  
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 «Национальный исследовательский Томский политехнический университет» (ТПУ)

Инженерная школа ядерных технологий  
Направление подготовки 14.04.02 Ядерные физика и технологии  
Отделение ядерно-топливного цикла

### МАГИСТЕРСКАЯ ДИССЕРТАЦИЯ

Тема работы
<b>Проект использования вертикального экспериментального канала большого диаметра реактора ИРТ-Т для нейтронного облучения полудрагоценных камней</b> УДК 621.039.55:539.125.5:671

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School of Nuclear Science and Engineering

Field of training (specialty) 14.04.02 Nuclear Science and Technology, Nuclear Power Installation Operation

Nuclear Fuel Cycle Division

### MASTER THESIS

<b>Topic of research work</b>
<b>The project on the application of the large diameter vertical experimental channel of the IRT-T reactor for neutron irradiation of semiprecious stones</b>

UDC 621.039.55:539.125.5:671

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Tomsk – 2020

Министерство науки и высшего образования Российской Федерации  
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 « \_\_\_\_ » \_\_\_\_\_ 2020

**ASSIGNMENT  
for the Graduation Thesis completion**

In the form:

Master Thesis
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For a student:

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Topic of research work:

Approved by the order of the Director of School of Nuclear Science & Engineering (date, number):	№129-4/c at 08.05.2020

Deadline for completion of Master Thesis:	01.06.2020
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**TERMS OF REFERENCE:**

<p><b>Initial date for research work:</b>  <i>(the name of the object of research or design; performance or load; mode of operation (continuous, periodic, cyclic, etc.); type of raw material or material of the product; requirements for the product, product or process; special requirements to the features of the operation of the object or product in terms of operational safety, environmental impact, energy costs; economic analysis, etc.)</i></p>	<ul style="list-style-type: none"> <li>– Reactor IRT-T with power of 6 MW;</li> <li>– Irradiation of semiprecious stones;</li> <li>– Computer simulation in MCU and COMSOL Multiphysics packages;</li> <li>– Maximum channel productivity;</li> <li>– Permissible level of induced activity 74 Bq\g.</li> </ul>
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<p><b>List of the issues to be investigated, designed and developed</b>  <i>(analytical review of literary sources with the purpose to study global scientific and technological achievements in the target field, formulation of the research purpose, design, construction, determination of the procedure for research, design, and construction, discussion of the research work results, formulation of additional sections to be developed; conclusions).</i></p>	<ul style="list-style-type: none"> <li>– Determination of a methodological approach to research of bulk solids physical system;</li> <li>– Determination of the optimal thickness of the thermal neutrons absorber for irradiation container;</li> <li>– Estimation of the permitted radius of irradiation container according to the calculated temperature conditions;</li> <li>– Evaluation of induced activity.</li> </ul>
<p><b>List of graphic material</b>  <i>(with an exact indication of mandatory drawings)</i></p>	<p>Presentation</p>

<p><b>Advisors to the sections of the Master Thesis</b>  <i>(with indication of sections)</i></p>	
Section	Advisor
<p>The project on the application of the large diameter vertical experimental channel of the IRT-T reactor for neutron irradiation of semiprecious stones</p>	<p>Artem G. Naymushin</p>
<p>Financial Management, resource efficiency and resource saving</p>	<p>Ekaterina V. Menshikova</p>
<p>Social responsibility</p>	<p>Dan A. Verigin</p>

<p><b>Date of issuance of the assignment for Master Thesis completion according to the schedule</b></p>	<p>05.02.2020</p>
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**Assignment issued by a scientific supervisor / advisor (if any):**

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**Assignment accepted for execution by a student:**

Group	Full name	Signature	Date
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## Task for section «Social responsibility»

To student:

group	Full name
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School	Nuclear Science and Engineering	Department	Nuclear fuel cycle
Degree	Master programme	Specialization	14.04.02 Nuclear physics and technologies

Title of graduation thesis:

<b>The project on the application of the large diameter vertical experimental channel of the IRT-T reactor for neutron irradiation of semiprecious stones</b>	
<b>Initial data for section «Social Responsibility»:</b>	
1. Information about object of investigation (matter, material, device, algorithm, procedure, workplace) and area of its application	Design of an experimental channel with the aim of using it at the IRT-T research nuclear reactor for irradiating semiprecious stones. Application area: industrial nuclear technologies.
List of items to be investigated and to be developed:	
<b>1. Legal and organizational issues to provide safety:</b> <ul style="list-style-type: none"> <li>– Special (specific for operation of objects of investigation, designed workplace) legal rules of labor legislation;</li> <li>– Organizational activities for layout of workplace.</li> </ul>	<ul style="list-style-type: none"> <li>– Labour code of Russian Federation #197 from 30/12/2001 GOST 12.2.032-78 SSBT</li> <li>– Sanitary Rules 2.2.2/2.4.1340-03. Hygienic requirements for PC and work with it</li> </ul>
<b>2. Work Safety:</b> 2.1. Analysis of identified harmful and dangerous factors 2.2. Justification of measures to reduce probability of harmful and dangerous factors	<ul style="list-style-type: none"> <li>– Enhanced electromagnetic radiation level</li> <li>– Insufficient illumination of workplace</li> <li>– Excessive noise</li> <li>– Deviation of microclimate indicators</li> <li>– Electric shock</li> </ul>
<b>3. Ecological safety:</b>	– Indicate impact of nuclear power plant on hydrosphere, atmosphere and lithosphere
<b>4. Safety in emergency situations:</b>	– Fire safety;

<b>Assignment date for section according to schedule</b>	05.02.2020
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**The task was issued by consultant:**

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Assistant professor	Verigin D.A.	Cand.of Sc.		

**The task was accepted by the student:**

Group	Full name	Signature	date
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**TASK FOR SECTION  
«FINANCIAL MANAGEMENT, RESOURCE EFFICIENCY AND RESOURCE SAVING»**

To the student:

Group	Full name
0AM8I	Brashchenko Andrey Aleksandrovich

School	Nuclear Science and Engineering	Division	Nuclear fuel cycle
Degree	Master	Educational Program	14.04.02 Nuclear physics and technologies

**Input data to the section «Financial management, resource efficiency and resource saving»:**

1. Resource cost of scientific and technical research (STR): material and technical, energetic, financial and human	– Salary costs – 154957.96 rub – STR budget – 249652.66 rub
2. Expenditure rates and expenditure standards for resources	– Electricity costs – 5,8 rub per 1 kW
3. Current tax system, tax rates, charges rates, discounting rates and interest rates	– Labor tax – 27,1 %; – Overhead costs – 30%;

**The list of subjects to study, design and develop:**

1. Assessment of commercial and innovative potential of STR	– comparative analysis with other researches in this field;
2. Development of charter for scientific-research project	– SWOT-analysis;
3. Scheduling of STR management process: structure and timeline, budget, risk management	– calculation of working hours for project; – creation of the time schedule of the project; – calculation of scientific and technical research budget;
4. Resource efficiency	– integral indicator of resource efficiency for the developed project.

**A list of graphic material** (with list of mandatory blueprints):

1. Competitiveness analysis
2. SWOT- analysis
3. Gantt chart and budget of scientific research
4. Assessment of resource, financial and economic efficiency of STR
5. Potential risks

**Date of issue of the task for the section according to the schedule**

**Task issued by adviser:**

Position	Full name	Scientific degree, rank	Signature	Date
Associate professor	E.V. Menshikova	PhD		

**The task was accepted by the student:**

Group	Full name	Signature	Date
0AM8I	Brashchenko Andrey Aleksandrovich		

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 «Национальный исследовательский Томский политехнический университет» (ТПУ)

School of Nuclear Science and Engineering  
Field of training (specialty) 14.04.02 Nuclear Science and Technology, Nuclear Power Installation Operation  
Level of education: Master degree programme  
Nuclear Fuel Cycle Division  
Period of completion: spring semester 2019/2020 academic year

Form of presenting the work:

Master Thesis
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**SCHEDULED ASSESSMENT CALENDAR  
for the Master Thesis completion**

Deadline for completion of Master’s Graduation Thesis:	01.06.2020
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Assessment date	Title of section (module) / type of work (research)	Maximum score for the section (module)
05.02.2020	Approval of the assignment	
01.03.2020	Review of the literature on the simulation of porous systems	
12.03.2020	Determination of the optimal thickness of the thermal neutrons absorber for irradiation container	
21.03.2020	Estimation of the permitted radius of irradiation	
28.03.2020	Evaluation of induced activity	
01.06.2020	Preparation of an explanatory note and submission of work and completion of Master’s thesis	

**COMPILED BY:**

**Scientific supervisor:**

Position	Full name	Academic degree, academic status	Signature	Date
Associate Professor	Artem G. Naymushin	PhD		

**AGREED BY:**

Programme Director	Full name	Academic degree, academic status	Signature	Date
Nuclear Power Installation Operation	Vera V. Verkhoturova	PhD		

*Expected learning outcomes*

Learning outcome (LO) code	Learning outcome (a graduate should be ready)	Requirements of the FSES HE, criteria and / or interested parties
<i>Professional competencies</i>		
LO1	To apply deep mathematical, scientific, socio-economic and professional knowledge for conducting theoretical and experimental research in the field of the use of nuclear science and technology.	FSES HE Requirements (PC-1,2, 3, 6, UC-1,3), Criterion 5 RAEE (p 1.1)
LO2	To demonstrate ability to define, formulate, and solve interdisciplinary engineering tasks in the nuclear field using professional knowledge and modern research methods.	FSES HE Requirements (PC-2,6,9,10,14, UC-2,3,4, BPC1,2), Criterion 5 RAEE (p 1.2)
LO3	To plan and conduct analytical, simulation and experimental studies in complex and uncertain conditions using modern technologies, and to evaluate critically research results.	FSES HE Requirements (PC-4,5,6,9,22, UC-1,2,5,6), Criterion 5 RAEE (p 1.3)
LO4	To use basic and special approaches, skills and methods for identification, analysis, and solution of technical problems in the field of nuclear science and technology.	FSES HE Requirements (PC-7,10,11,12,13, UC-1-3,BPC1,3), Criterion 5 RAEE (p 1.4)
LO5	To operate modern physical equipment and instruments, to master technological processes in the course of preparation for the production of new materials, instruments, installations, and systems.	FSES HE Requirements (PC-8,11,14,15, BPC-1), Criterion 5 RAEE (p 1.3)
LO6	To demonstrate ability to develop multioption schemes for achieving production goals with the effective use of available technical means and resources.	FSES HE Requirements (PC-12,13,14,16, BPC-2), Criterion 5 RAEE (p 1.3)
<i>Cultural competencies</i>		
LO7	To demonstrate ability to use a creative approach to develop new ideas and methods for designing nuclear facilities, as well as to modernize and improve the applied technologies of nuclear production.	FSES HE Requirements (PC-2,6,9,10,14, UC-1,2,3), Criterion 5 RAEE (p 1.2,2.4,2.5)
<i>Basic professional competencies</i>		
LO8	To demonstrate skills of independent learning and readiness for continuous self-development within the whole period of professional activity.	FSES HE Requirements (PC-16,17,21, UC-5,6, BPC-1), Criterion 5 RAEE (p 2.6) coordinated with the requirements of the international standard EURACE & FEANI
LO9	To use a foreign language at a level that enables a graduate to function successfully in the international environment, to develop documentation, and to introduce the results of their professional activity.	FSES HE Requirements (BPC-3, UC-2,4), Criterion 5 RAEE (p 2.2)



LO10	To demonstrate independent thinking, to function efficiently in command-oriented tasks and to have a high level of productivity in the professional (sectoral), ethical and social environments, to lead professional teams, to set tasks, to assign responsibilities and bear liability for the results of work.	FSES HE Requirements (PC-18,20,21,22,23, UC-1,4, BPC-2), Criterion 5 RAEE (p 1.6,2.3) coordinated with the requirements of the international standard EUR-ACE & FEANI
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## **Abstract**

The final qualification work in the form of Master's thesis contains 97 pages, 10 figures, 21 tables, 32 references, 2 appendices.

Keywords: topaz, semiprecious stones, radiation treatment, crystal defects, porous system, nuclear reactor, fast neutron flux, experimental channel.

Object of this research is project on the application of the large diameter vertical experimental channel of the IRT-T reactor for neutron irradiation of semiprecious stones

The goal of this work is to determine and optimize operating conditions for using the vertical experimental channel of a large diameter IRT-T reactor for neutron irradiation of semiprecious stones.

As a result of the study, the possibility of implementing the radiation treatment technology of semiprecious stones in the designed vertical experimental channel of the IRT-T reactor using the example of topazes is studied. The optimal thickness of the thermal neutron absorber in the container for irradiation, corresponding to the required neutronic characteristics when irradiating semiprecious stones, made of boron carbide with thickness of 3 mm, is determined. The temperature conditions in the irradiated container are calculated and the conclusion about reducing the useful radius of the container from 10.2 cm to 7.2 cm is drawn. The induced activity of the irradiated semiprecious stones is estimated.

Scope: nuclear technologies. Economic efficiency and importance of the research work is high.

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## **Introduction**

It is known that deposits of naturally colored semiprecious stones in nature are practically depleted, and the demand for them is growing. Therefore, at present, radiation technologies are used to color these crystals. The most common semiprecious stone used in this technology is topaz. Neutron irradiation is used to give topaz various shades of blue (from light blue to dark blue), which increases its jewelry value several times. In the process of irradiation with fast neutrons in the topaz crystal, structural defects are formed that change its optical properties.

Research nuclear reactors have great potential as a tool for the radiation treatment of topaz crystals. However, this technology is far from perfect and requires a large amount of research and work.

From this we can conclude that in order to create and continue normal operation of the installation for irradiating semiprecious stones on the new projected channel of the IRT-T research reactor, a number of studies are necessary.

First of all, it is necessary to consider the physical laws of calculating bulk solids physical system, an example of which is the filling of topazes in an irradiation container. It is necessary to consider the basic physical quantities characterizing such systems, including the dependence of the thermal conductivity of the system on the shape and size of particles in the bulk, as well as the change in thermal conductivity with increasing temperature during irradiation.

After that, it is necessary to evaluate whether the working conditions in the designed channel correspond to the required ones: irradiation of topazes requires fast neutrons (which entails the need to use an optimal filter system for thermal neutrons). It is necessary to create a model of an irradiation container with samples and determine the optimal material composition of the filtering system.

It is known that when semiprecious stones are irradiated with neutrons, volumetric energy release occurs. In addition, it is known that at sufficiently high temperatures, annealing of defects in crystals, as well as their cracking, is observed, which nullifies the results of stone irradiation. Thus, the next step is to determine the

allowable radius of the container, at which compliance with the permissible temperature conditions during irradiation will be observed.

The last stage of the study will be the determination of the induced activity in the samples after their irradiation. In this case, it is necessary to determine what impurity elements are present in the minerals, then simulate their irradiation in the reactor, and determine the delay time for the stones after irradiation before their use by consumers.

Thus, the goal of this work is to determine and optimize operating conditions for using the vertical experimental channel of a large diameter IRT-T reactor for neutron irradiation of semiprecious stones. Based on the stated goal, the following tasks were set:

- Determination of a methodological approach to research of bulk solids physical system.
- Determination of the optimal thickness of the thermal neutron absorber in the container for irradiation, corresponding to the required neutronic characteristics when irradiating semiprecious stones;
- Estimation of the permitted radius of irradiation container according to the calculated temperature conditions;
- Evaluation of induced activity of the irradiated semiprecious stones and delay time for irradiated stones before usage by consumers.

## **1 Determination of a methodological approach to research**

The research reactor IRT-T is a pool-type thermal reactor using distilled water as a moderator, coolant and biological protection. The reactor is a powerful source of neutron and gamma radiation and is intended for scientific research in the field of nuclear physics, solid-state physics, radiobiology, and solving applied problems in the field of ecology and medicine. The reactor was commissioned in 1967, its thermal capacity is 6 MW [1].

The reactor core is assembled from fuel assemblies of the IRT-3M type, and the number of fuel assemblies and the configuration of the core, as well as the composition of the reflector, can be changed. The reactor has special experimental devices called experimental channels. This is a complex of equipment and devices of the reactor, combined into one system, designed for experimental research on the reactor.

The experimental channels of research nuclear reactors have great potential as a tool for radiation processing of materials. Currently, experience has been gained in their successful application in many technologies for the modification of solids: in the production of materials with desired properties, in the manufacture of radiopharmaceuticals for the diagnosis and treatment of various diseases, for neutron activation analysis of specimens, etc.

Especially important here is the potential of the experimental channels of research reactors for the implementation of neutron transmutation doping (NTD) technologies for silicon ingots. In NTD, dopants are not inserted into the semiconductor, but are formed from silicon atoms under the influence of a thermal neutron flux. From the  $\text{Si}^{30}$  silicon isotope, the  $\text{Si}^{31}$  radioactive isotope is formed, which then decays to form the stable phosphorus isotope  $\text{P}^{31}$  with n-type conductivity. NTD allows to obtain single-crystal silicon with a particularly uniform distribution of impurity atoms.

At present, a new vertical large-diameter experimental channel [2] is being put into operation at the IRT-T reactor, designed for alloying silicon ingots with a large

diameter of 20.4 cm. Obviously, there is a need to maximize the economic potential of this channel, and therefore the entire reactor, for irradiation of samples. Therefore, due to the inconstancy of the use of the channel for NTD, it is necessary to develop a technology for the alternative use of this vertical experimental channel in order to use it at time intervals when silicon is not irradiated, and evaluate its technical capabilities.

So, it is known that in addition to silicon, which is fundamentally important for power electronics, other materials can be irradiated in experimental channels, a special place among which is a group of so-called semiprecious stones. Semi-precious stones are minerals used in jewelry, but occurring in nature much more often than precious stones. Such minerals include amethyst, aquamarine, chrysolite, quartz, agate, etc. A special place among these minerals is occupied by topaz, as one of the most popular semiprecious stones.

Due to the fact that deposits of natural colored topazes are practically depleted, and the demand for these semiprecious stones is growing, there is a need to expand the technology for modifying the optical properties of colorless natural minerals using ionizing radiation. Thus, in the study under consideration, a project is proposed for the alternative use of a vertical experimental channel for irradiating semiprecious stones in it. The study is conducted on the example of the most popular semiprecious stone used to modify optical properties - topaz.

Topaz is a mineral from the group of aluminum silicates having the chemical formula  $\text{Al}_2(\text{F},\text{OH})_2\text{SiO}_4$ . All colors inherent in topaz, except for violet, have a radiation nature, while the violet color is due to ions  $^{+3}\text{Cr}$ , isomorphically substituting  $^{+3}\text{Al}$  in the structure of the mineral. If topazes are free of impurities and defects, they should be colorless. In nature, topaz generally occurs as yellow or yellow brown, pale blue as well as colorless. When it is heated, yellow topaz often becomes orangy pink. Natural pink topaz, however, is extremely rare; this color is usually obtained by heating certain yellow to reddish brown Brazilian material that contains the chromium required to produce pink. In general, the scheme of color change under the influence of radiation exposure and heating is presented in Figure 1 [3].



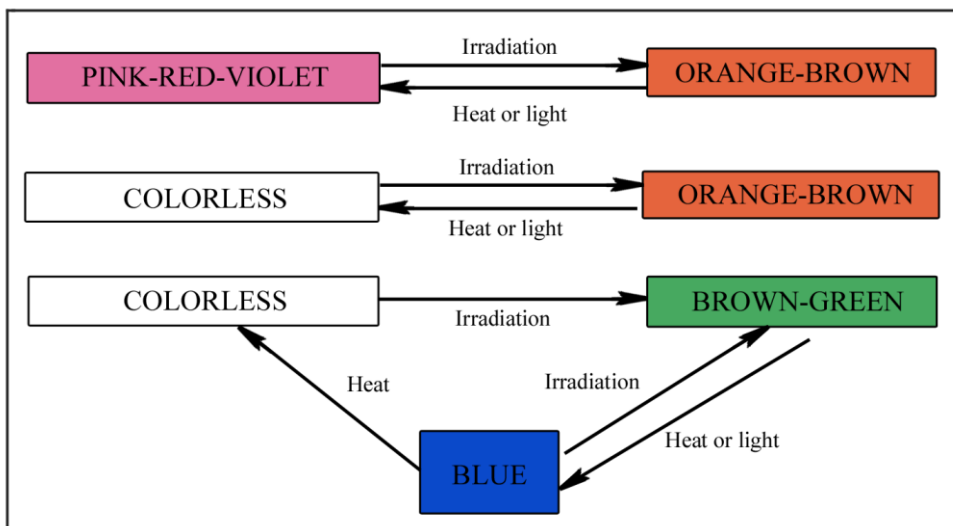


Figure 1 – Scheme of color change

As can be seen from the figure, irradiation is used to give topaz various shades of blue. Several types of irradiation can be used to alter the color in topaz: gamma rays, neutrons, and high-energy charged particles such as electrons, protons, and the like. The neutrons in a nuclear reactor can be of varying energy and are also accompanied by gamma rays and other rays and particles. Therefore, during the irradiation, both the brown and the blue colors in topaz can be produced, and heating is used to remove the brown if blue is desired. Figure 2 shows photographs of topazes before irradiation, after irradiation in the reactor with a fast neutron flux, having shades of brown and blue, as well as after their subsequent heating. Topazes after heating and control of induced radioactivity can be used by consumers.



Colorless, before irradiation

Blue-brown, after irradiation

Swiss blue, after heating

Figure 2 – The effects of radiation and heating on topaz

Currently, blue topaz on the market is classified according to the shade of blue as Sky blue, Swiss blue and London blue, shown in figure 3.



Figure 3 – Shades of blue topaz

Thus, in the process of irradiation with fast neutrons in the topaz crystal, structural disturbances are formed that change its optical properties. These topazes in their optical properties are indistinguishable from natural colored topazes, including optical absorption spectra. In the process of neutron irradiation, both simple and complex defects of the crystal lattice (defect complexes) arise in the crystal structure of topazes. The defect complexes form the electron and hole color centers.

Obviously, when creating a technology for modifying the optical properties of topazes, it is desirable to have the highest possible productivity of the irradiation channels, the lowest specific activity of the minerals, as well as the acceptable temperature of the minerals when they are irradiated, at which cracking and cloudiness of the crystals and annealing of radiation defects would not occur.

However, the fulfillment of one condition leads to negative consequences for another. For example, increasing productivity by increasing the volume of containers leads to an increase in temperature in the container, as well as an increase in the activity of minerals. A decrease in temperature due to cooling of the container with water leads to a loss of the fast neutron flux density and to an increase in the activity of minerals due to additional generation of thermal and especially resonant neutrons. It follows from this that there are three important factors that must be taken into account when creating an irradiation device: productivity, irradiation temperature, and topaz radioactivity after irradiation. It is also worth noting that the first step in the study is to check whether the implementation of this technology in this experimental channel is possible.

Thus, it is required to analyze the neutron-physical conditions in the channel and their applicability to the irradiation of semiprecious stones; calculate the temperature conditions during irradiation and draw a conclusion about the maximum channel productivity; in addition, it is necessary to calculate the induced activity in the stones after their irradiation and to evaluate the exposure time of the stones before their use by consumers. After this, the task is to optimize the working conditions, which includes reducing the non-uniformity of the exposure, as well as increasing the productivity with decreasing the induced activity.

In this work, the calculations were performed using the Monte Carlo Universal (MCU) software. Monte Carlo Universal is a project for the development and practical use of a universal computer program for numerically simulating the processes of the transfer of various types of radiation (neutrons, gamma rays, electrons) in three-dimensional systems using the Monte Carlo method (the Monte Carlo method refers to a numerical method for solving mathematical problems with modeling random variables).

The advantages of the Monte Carlo method are that it allows to simulate the interaction of radiation with matter based on information from files of estimated nuclear data and practically does not impose restrictions on the geometry of the systems under consideration [4]. In many cases, the Monte Carlo method, together with the estimated nuclear data, can successfully replace the experiment. This class of programs is finding wider application in the analysis of radiation and nuclear safety of existing and in the design of new facilities for the use of atomic energy in other applications. The MCU program code is widely used throughout the world for neutronic calculations of research nuclear reactors, although it can be used for most thermal reactor gratings.

This software was chosen due to the possibility of accurate analysis of ongoing processes in the reactor and the absence of the requirement for extensive knowledge of all user options of the MCU package for user. There is a created calculation model of the IRT-T reactor core, created by means of the Monte Carlo Universal package. The approach set in the program allows to describe in detail the geometric characteristics and take into account the heterogeneity of the structure of the reactor core.

Thus, based on the existing model of the IRT-T reactor in MCU code, first it is necessary to simulate the installation for the irradiation of semiprecious stones. Before modeling such an irradiation system for topaz treatment, it is necessary to consider the physical laws of porous systems, which is a filling of irradiated stones in container. It is also necessary to analyze the structural composition of topaz, as well as the effect of the presence of a gas component between the samples on heat transfer during irradiation.

## 2 Basing of the calculation model

As mentioned earlier, in this study, neutronic and thermal-hydraulic calculations of a new vertical experimental channel of large diameter, designed for doping of silicon ingots, with a view to its alternative use for irradiation of semiprecious stones, are performed. The first step of the study is to consider the laws and general physical principles applied to the simulation and calculation of so-called porous physical systems which consist of particulate solids in bulk, examples of which are irradiated stones filled in container. Based on these physical principles subsequent calculations in the study are made.

### 2.1 Modeling of porous physical systems

The scheme of the experimental channel considered in this work is presented in Figure 4.

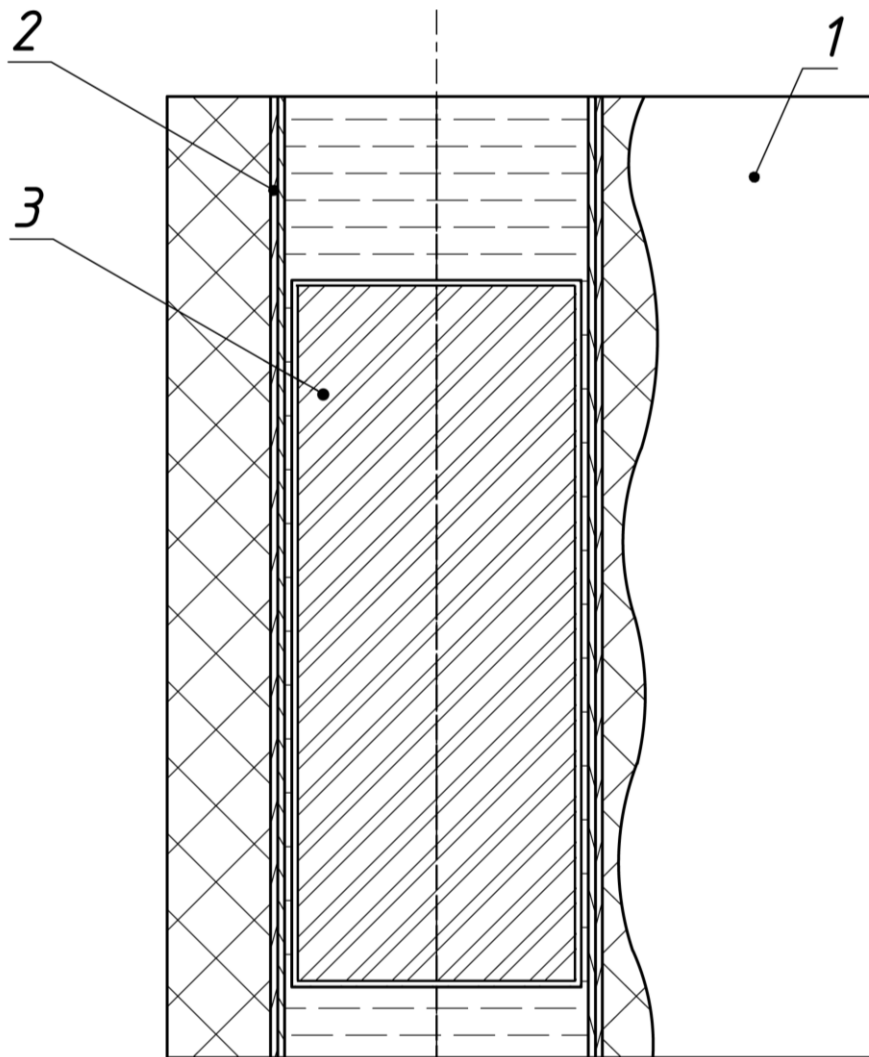


Figure 4 – Cross-section of the considered vertical channel

The designed channel is intended for doping silicon with a diameter of up to 10.2 cm and heights of 50 cm with a flux of thermal neutrons. The system contains a graphite box 1 located near the reactor core. A vertical hollow aluminum cylinder 2 with a filter system is placed in the box. The filter system consists of a boron carbide compound sprayed over the height, the concentration of which is selected so as to achieve the smallest axial and radial non-uniformity of doping in the irradiation volume. The height of the channel is 70 cm, the inner diameter is 10.7 cm. The channel is filled with water intended for cooling silicon ingots.

In this paper, a project is proposed for using this channel for irradiation of semiprecious stones. To do this, in the considered channel, the container with silicon 3 is replaced by the container with the studied material. The most common material used in this technology is topaz crystals. The required irradiation results are achieved by irradiating the samples with a fast neutron flux.

The first step in creating a calculation model is to determine the structural properties of the irradiated material. In the study of numerous samples of topaz, it was found that the average structural formula for a molecule of a topaz crystal has the following form [5]:



In addition, the presence of impurities in topazes that play an important role in the induced activity of materials should be taken into account. Studies in the analysis of various samples from various deposits show [5–7] that the main impurities in the mass content in topaz are  $\text{Li}^7$ ,  $\text{Ca}^{44}$ ,  $\text{Ti}^{47}$ ,  $\text{V}^{51}$ ,  $\text{Cr}^{52}$ ,  $\text{Fe}^{56}$ ,  $\text{Ga}^{71}$ ,  $\text{Cs}^{133}$ ,  $\text{Ta}^{181}$  and a number of other impurities. The density of topazes is taken equal  $\rho=3.5 \text{ g/m}^3$ . Based on this, concentrations of elements necessary for further calculation are calculated. The main role in modeling of container with topazes and further calculating of operating conditions during irradiation the fact is played that the irradiated semiprecious stones are the so-called porous system, which consists of solid and gas phases. The solid phase is stones, the gas phase is air inter the stones in the bulk. In general, the topaz bulk in the container can be represented as shown in Figure 5.

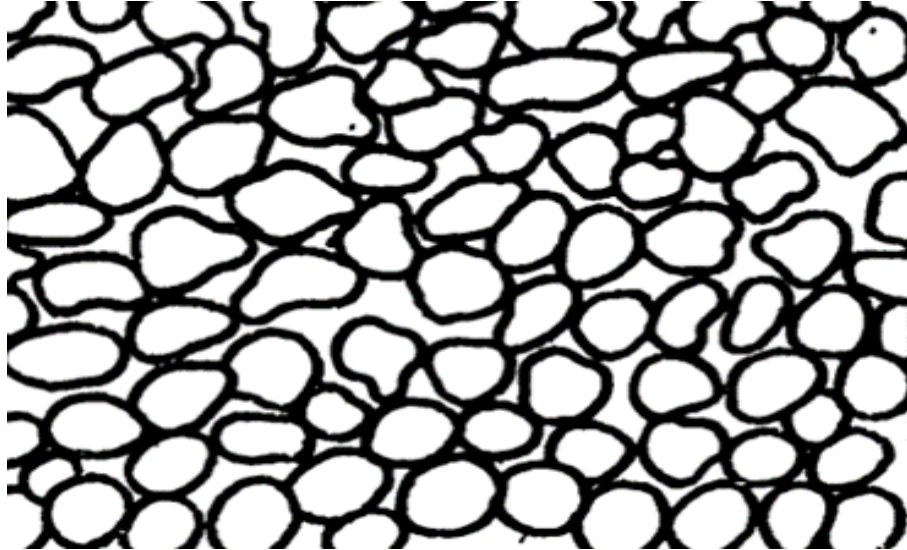


Figure 5 – Representation of topaz bulk

Thus, it is obvious that when simulating heat transfer in a container, it is necessary to take into account the dependence of the thermal conductivity of the whole system and element concentrations on the density of the bulk. In the general case, any bulk is characterized by the porosity  $m$ :

$$m = 1 - \frac{\rho_{bulk}}{\rho_0} = \frac{V_g}{V_s + V_g}$$

where:  $\rho_{bulk}, \rho_0$  – bulk density and solid phase density;

$V_s, V_g$  – volumes occupied by solid and gas phases.

Without experimental data, the porosity of the bulk can be approximately determined from the dependence for the averaged particle size in bulk [8], where the topaz bulk system shown in Figure 5 is replaced by a bulk system of particles (stones) with averaged size. According to [3,9], topazes weighing from 5 to 50 carats are irradiated in reactors, however, most often samples weighing about 10 carats are subject to irradiation [10-11], which is equivalent to 2 grams. A ball-shaped stone of topaz with such mass and density of topaz will have a radius:

$$R = 3 \sqrt{\frac{3}{4\pi} \frac{m}{\rho}} = 5.14 \text{ mm} \approx 5 \text{ mm},$$

where:  $m$  – mass of such averaged sphere;

$\rho$  – topaz density.

Then, according to [8], for such a value of the averaged radius, the porosity can be taken equal to  $m = 0.33$ . Then, the density of the bulk will be equal  $\rho_{bulk} = 0.67\rho_0 = 2.345 \text{ g/cm}^3$ . After that, the concentrations of elements necessary for further calculation are recalculated.

For further thermal-hydraulic and neutron-physical calculations in the MCU software package, detailed model of the experimental channel under consideration was created on the basis of the existing IRT-T reactor model. This model is presented in Figure 6: on the left picture is a vertical cross-section of the channel, on the right is the location of the channel under consideration relative to the reactor core.

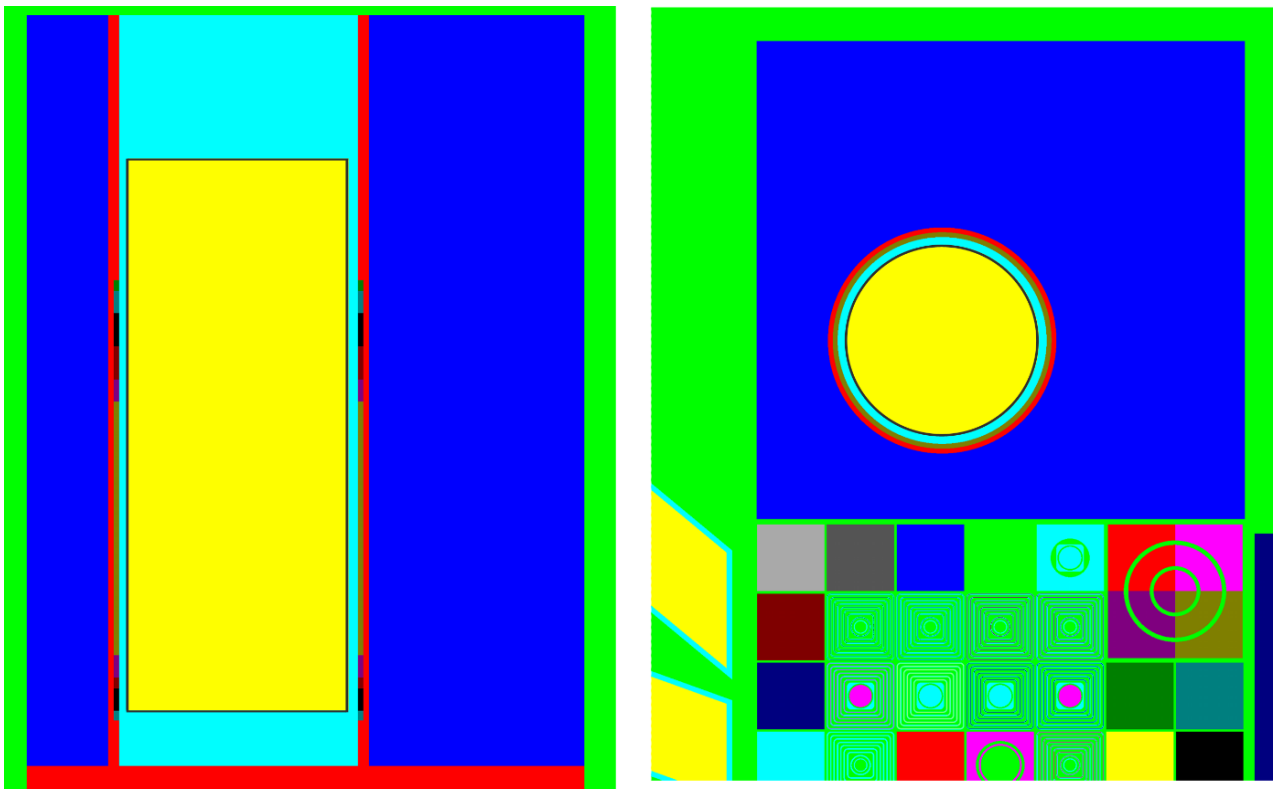


Figure 6 – Model of the experimental channel in the MCU software

Silicon material is replaced with topaz material taking into account porosity, concentrations of the main elements and impurity elements are introduced, a container is added, which also plays the role of a thermal neutron absorber; Initially, the container is made of aluminum, later in the calculations the container is made of a thermal neutron absorber, and its thickness and material are calculated.



Further, when calculating the energy release during irradiation, it is necessary to use in calculations the value of the thermal conductivity coefficient of topazes. Obviously, the value of the thermal conductivity coefficient for bulk will have a completely different value, in contrast to a solid system due to the presence of air in the pores. In this case, the value of the so-called effective thermal conductivity coefficient of the entire system is operated, which takes into account the influence of the gas and solid phases, porosity, size and shape of the particles in the bulk, etc. Let's consider different researches which consider some models of determining the effective thermal conductivity of the bulk.

## **2.2 Determination of the effective thermal conductivity of the bulk**

There are different models to determine the value of the effective coefficient of thermal conductivity, having different accuracy, some of them require experiments, and others are theoretical. Moreover, in the present work, in the absence of experimental data, a method based purely on geometric considerations is required, yielding acceptable results for taken value of porosity, while being a function of the porosity and thermal conductivity of the gas and solid phases:

$$\lambda_{eff} = f(m, \lambda_s, \lambda_g)$$

One of the methods is simple method of “averaging” the size of particles in the bulk. This method is similar to the method for determining the porosity of the considered system: it is assumed that the particles in bulk have the same shape and the same size, then a unit cell for the system is selected, effective thermal conductivity coefficients for the beds are calculated. Then size and particle shape corrections are introduced giving acceptable results for calculating real bulk.

To determine the effective thermal conductivity of the bulk of topazes subjected to irradiation, it is necessary to know the temperature dependence of the thermal conductivity of topaz and air. To determine the thermal conductivity of topazes at various temperatures, references were analyzed [12-14], and the thermal conductivities of topazes at various temperatures were determined. The obtained values are listed in Table 1.

Table 1 – Thermal conductivity of topaz of different temperatures

$t, ^\circ\text{C}$	$\lambda, \text{W/mK}$
0	21.565
25	18.660
38	18.680
42	17.700
85	15.600
93	16.258
144	13.003
149	13.664

Thus, by plotting the dependence of the coefficient of thermal conductivity on temperature, we can analytically determine the law of change in thermal conductivity. The dependence of the thermal conductivity coefficient on temperature and the approximating curve are presented in Figure 7.

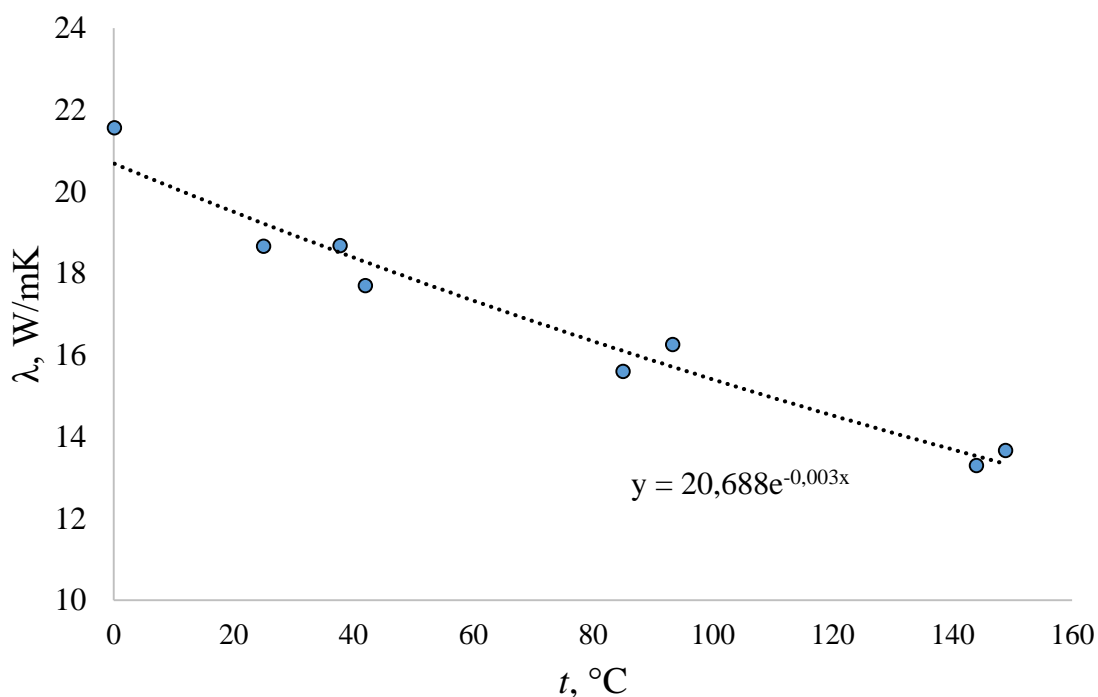


Figure 7 – Thermal conductivity of topaz monocrystal

It is known that heat transfer in any medium is due to heat conduction, convection, and radiation. For the solid phase, the heat transfer when the temperature changes depends only on the thermal conductivity, then for the gas phase it is necessary to take into account the contribution to the thermal conductivity of the radiation component:

$$\lambda_g = \lambda_{cond} + \lambda_{rad}$$

As shown in [15], the radiation component of thermal conductivity depending on the temperature of the air phase in the container can be determined from the following relationship:

$$\lambda_{rad} = 4 \cdot \varepsilon \cdot \sigma \cdot d_c \cdot T^3$$

where  $\varepsilon$  – emissivity of material (topaz);

$\sigma$  – Stefan–Boltzmann constant  $\sigma = 5.67 \cdot 10^{-8} \text{ kg s}^{-3} \text{ K}^{-4}$ ;

$T$  – temperature, K;

$d_c$  – the average pore diameter in the bulk, m.

The value of emissivity for aluminosilicates is in the range of 0.9–0.95 [16]; for the calculations, the value  $\varepsilon = 0.95$ . The average pore diameter in the bulk  $d_c$  can be found by interpolation if the dependence of the pore size on the average particle size in a bed with an ideal cubic packing with a porosity of  $m=0.476$  and tetrahedral packing with porosity  $m=0.259$  are known. The dependence of the average pore diameter in the bulk on the average particle diameter in the bulk, which is taken  $d_p = 1 \text{ cm}$ , for cubic and tetrahedral packing is determined from [17], and using interpolation the average pore diameter for bulk with porosity  $m = 0.33$  is found, is equal 4.2 mm.

Thus, the dependence of the thermal conductivity of air on temperature is plotted, as shown in Figure 8.

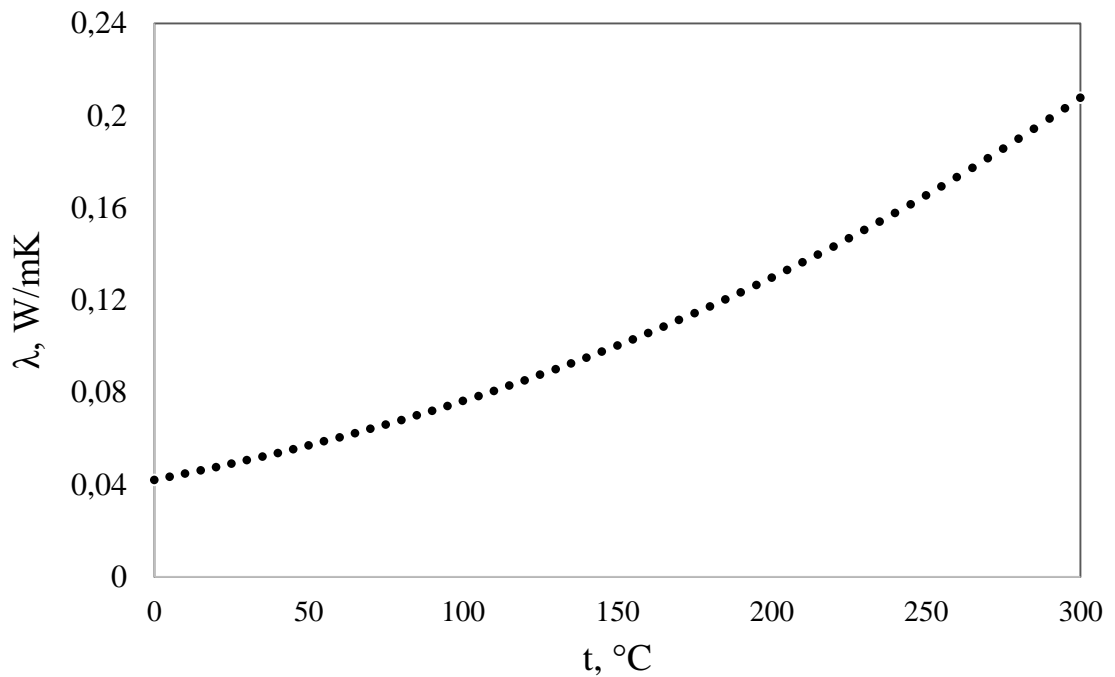
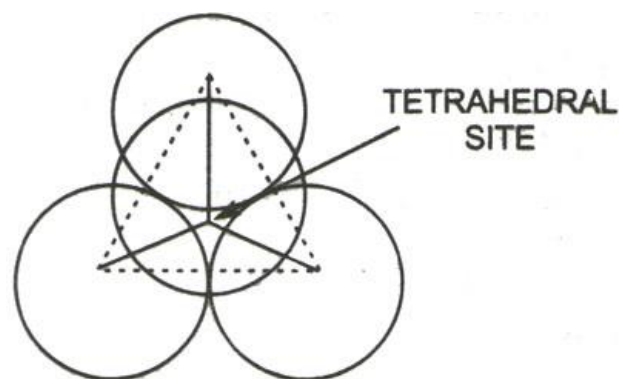


Figure 8 – Thermal conductivity of air with temperature increase

Knowing the temperature dependence of the thermal conductivity of air and topazes, it is possible to determine the value of the effective thermal conductivity coefficient. Let us consider several models. In the first model of V.Z. Bogomolov [18], based on the so-called tetrahedral approximation described in [8], it is assumed that the bulk under consideration is replaced by another bulk with equivalent thermal conductivity, where the size-averaged particles have a tetrahedral packing, shown in Figure 9.



A tetrahedral-interstices

Figure 9 – Tetrahedral unit cell

The value of thermal conductivity can be approximately determined using the following formula:

$$\lambda_{eff} = \frac{3\pi}{k} \cdot \lambda_g \cdot \left[ \frac{1}{k} \cdot \ln \left( \frac{1 - 0.82 \cdot \frac{r}{b} \cdot k}{1 - k \cdot \frac{r}{b}} \right) - 0.09 \cdot \frac{r}{b} \right]$$

where:  $r$  – average particle radius;

$$k = 1 - \frac{\lambda_g}{\lambda_s}$$

$\lambda_g$  – thermal conductivity of the gas phase (air) in the bulk;

$\lambda_s$  – thermal conductivity of the solid phase;

$b$  – radius dependent geometric parameter  $b = r + a$ .

Moreover, for geometric reasons, the value of  $a$  can be associated with porosity:

$$\frac{a}{r} = \frac{m - 26}{3 \cdot (100 - m)}$$

Here  $m$  – in percents.

The formula gives an error of up to 15%, which is an acceptable result for a model built only on geometric considerations without any experimental studies.

Another method for determining the effective thermal conductivity of the bulk, based on the value of porosity, is considered in the work of Kunii and Smith [19–20]. We also consider a system equivalent to real bulk, consisting of random packing of balls with porosity  $m$ . The formula for effective thermal conductivity will have the following form:

$$\lambda_{eff} = \lambda_g \left[ m + \frac{1 - m}{\varphi + \frac{2 \lambda_g}{3 \lambda_s}} \right]$$

where:  $m$  – value of porosity;

$\lambda_s$  – thermal conductivity of the solid phase in the bulk;

$\lambda_g$  – thermal conductivity of the gas phase (air) in the bulk;

$\varphi$  – coefficient determining heat transfer at the points of contact of grains of bulk, the value of which is determined from the following formula:

$$\varphi = \varphi_2 + (m - 0.259)(\varphi_1 - \varphi_2) / 0.217$$

Where the coefficients  $\varphi_1$  and  $\varphi_2$  the coefficients are defined as functions of the deviation of the thermal conductivity of the solid and gas phases  $\varphi_i = f\left(\frac{\lambda_s}{\lambda_g}\right)$  from perfect cubic packing  $m_1=0.476$  and ideal tetrahedral packing  $m_2=0.259$  and are determined from the complex graphical dependence described by Kunii and Smith in [20].

Another way to determine the effective thermal conductivity is the method described by Zehner and Schlunder [19,21]. They considered for the unit cell one-eighth of a cylinder (inner cylinder of unit radius and outer cylinder of radius  $R$ ). Fluid is filled between the inner and outer cylinders while the inner cylinder consists of both the solid and the fluid phases.

The formula for determining the effective thermal conductivity is as follows:

$$\lambda_{eff} = \lambda_g \left[ 1 - \sqrt{1-m} + \frac{2\sqrt{1-m}}{1-kB} \left( \frac{(1-k)B}{(1-kB)^2} \ln\left(\frac{1}{kB}\right) - \frac{B+1}{2} - \frac{B-1}{1-kB} \right) \right]$$

where  $k = \frac{\lambda_g}{\lambda_s}$  – the ratio of the gas phase in the bulk to solid;

$B$  is the porosity depended shape factor characterizing the geometrical effect of the solid particle. For  $B \rightarrow 0$ , the system becomes with no solid volume; for  $B \rightarrow \infty$  the solid occupies the entire inner cylinder:

$$B = C \left( \frac{1-m}{m} \right)^{10/9}$$

The constant  $C$  depends on the shape of the particle. Zehner and Schlunder suggest that  $C=1.25$ ,  $1.40$  and  $2.5$  for spheres, broken (irregular particles) and cylinders respectively.

Using the considered models, the thermal conductivities of the solid and gas phases were calculated, and the effective thermal conductivities for each case were

determined. Certain dependences of the effective thermal conductivity on temperature, as well as their averaged curve are shown in Figure 10.

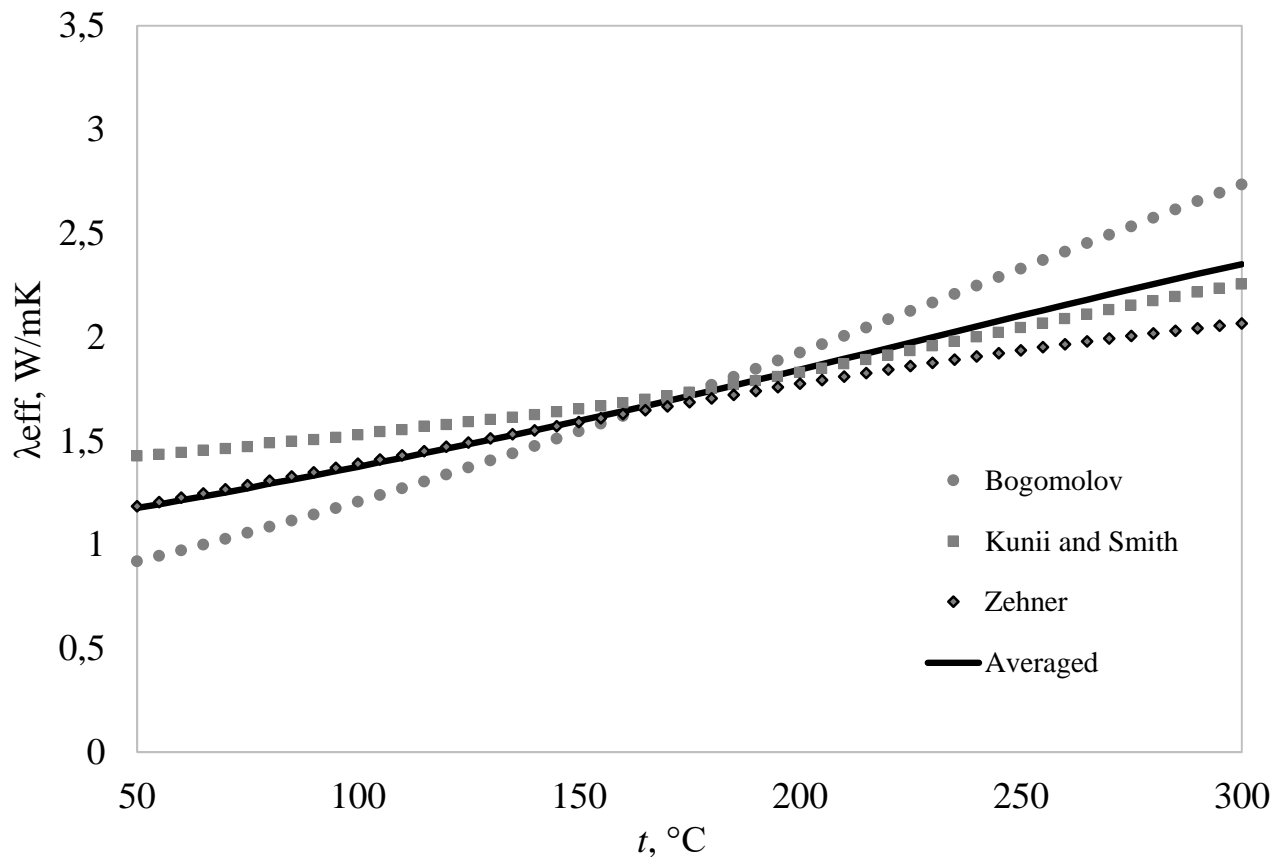


Figure 10 – Effective thermal conductivity of bulk

In this case, the approximating dependence has the following form:

$$\lambda_{eff} = 0.004559 \cdot t + 0.949387$$

It can be seen that, in general, the presence of air significantly reduces the value of the thermal conductivity coefficient, however, with increasing temperature, the thermal conductivity coefficient of the bulk increases due to an increase in the thermal conductivity of air due to convection and due to an increase in the radiation component of the heat flux.

In addition, further calculations should take into account the change in thermal conductivity of the material of the container for irradiating topazes. It is known that a container for irradiating topazes is made of a material that absorbs thermal neutrons, such as cadmium or boron carbide.

The next step in the study is to calculate the average neutron flux in the container and determine the configuration of the filter system, in particular the thickness and material of the filter, as well as study the temperature conditions in the container and calculate the induced activity in topazes upon irradiation.



### 3 Determination of operating conditions in irradiated container

As mentioned earlier, when creating a technology for modifying the optical properties of topazes, it is desirable to have the highest possible productivity of the irradiation channels, the lowest induced specific activity of the minerals and the acceptable temperature of the minerals when they are irradiated. Accordingly, the productivity of the modification of minerals depends on the volume of minerals in the container, on the neutron flux density and on the neutron spectrum. The harder the spectrum of neutrons, the higher the defect formation and productivity. To harden the spectrum in existing installations for the irradiation of semiprecious stones, containers for irradiation using thermal neutron filters are used [22-24,32]. As a filter, materials are used that actively absorb thermal neutrons, such as boron carbide or cadmium.

Thus, the next step in the study is to determine whether the existing operating conditions on the projected channel correspond to those required during gemstones irradiation. Otherwise, it is necessary to consider the use of a thermal neutron filter and determine its necessary configuration.

It is known that the most common material used in this technology is a topaz crystal. Radiation coloring is associated with the formation of defects in the crystal structure under the influence of ionizing radiation. Studies have shown that the effective energy for the formation of necessary defects starts at 0.5 MeV, the concentration of defects increases with increasing neutron energy and reaches saturation at a neutron energy of 1 MeV [1, 22-23]. In many implemented technologies on semiprecious stones treatment, 1 MeV is taken as the fast neutron energy boundary [1, 22-25].

Studies show [22-24] that the ratio of the average fast neutron flux to the average thermal neutron flux should be  $k = \frac{\overline{\Phi}_f}{\overline{\Phi}_{th}} \geq 10$ , which would provide the best conditions for the irradiation of samples. In this case, the energy of 1 MeV is taken as the boundary of fast neutrons.

Thus, for further research it is necessary to determine whether the necessary condition for the fast to thermal flux ratio will be satisfied for the existing geometry and the required boundaries of the energy groups. Therefore, in this paper, we consider the distribution of the neutron flux over the height of the container. In particular, groups of fast and thermal neutrons for various thermal neutron filters are considered.

### 3.1 Creating a working model

In the general case, the model of the installation under consideration has the form shown in Figure 11. In the MCU program, based on this, a calculation model was created with a detailed study of the experimental channel.

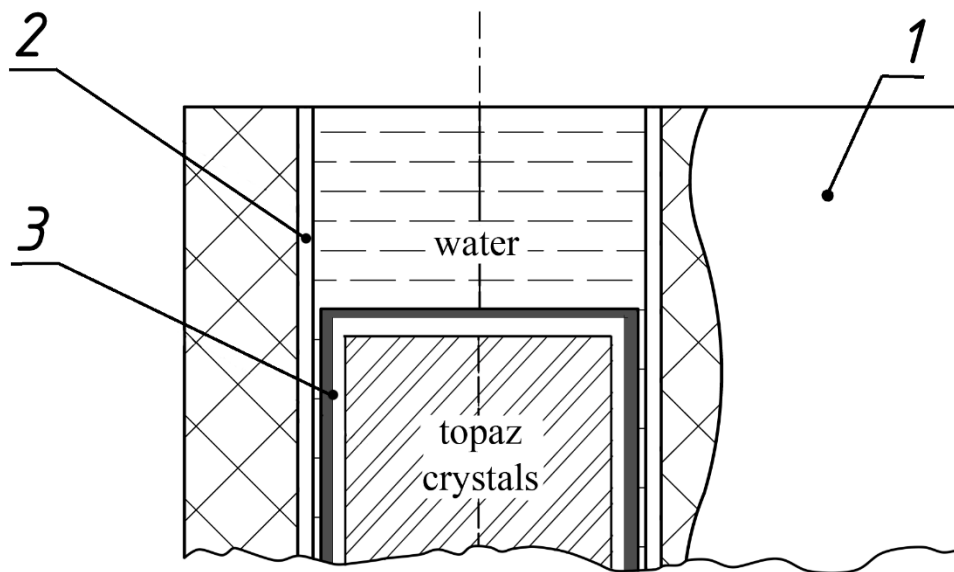


Figure 11 – Scheme of the container with irradiated topaz

In the center of the channel, which made in the form of a hollow aluminum cylinder 2 placed in a graphite prism 1, there is a container with topaz 3. At the initial stage of the study, its volume is equivalent to the volume of a container with silicon: height is 50 cm, outer diameter is 20.4 cm. The walls of the container are made of aluminum; the container is wrapped with cadmium foil or contains boron carbide, which play the role of a thermal neutron filter. In general, the absorber is shown in gray in the figure.

The effective volume of the container (volume with crystals of topaz) is divided into objects (cylinders) with height of 1 cm and the value of the neutron flux is

determined in each object. The energy boundaries were 1 MeV for fast neutrons and 0.625 eV for thermal neutrons.

First, we take the initial wall thickness of the container equal to 1 mm, while the walls of the container are made of aluminum, without using an absorber, and the container is filled with topazes. The calculations carried out using the MCU software and considered for thermal and fast neutron groups. The resulting distribution of the average value of the neutron flux over the height of the container is presented in Figure 12.

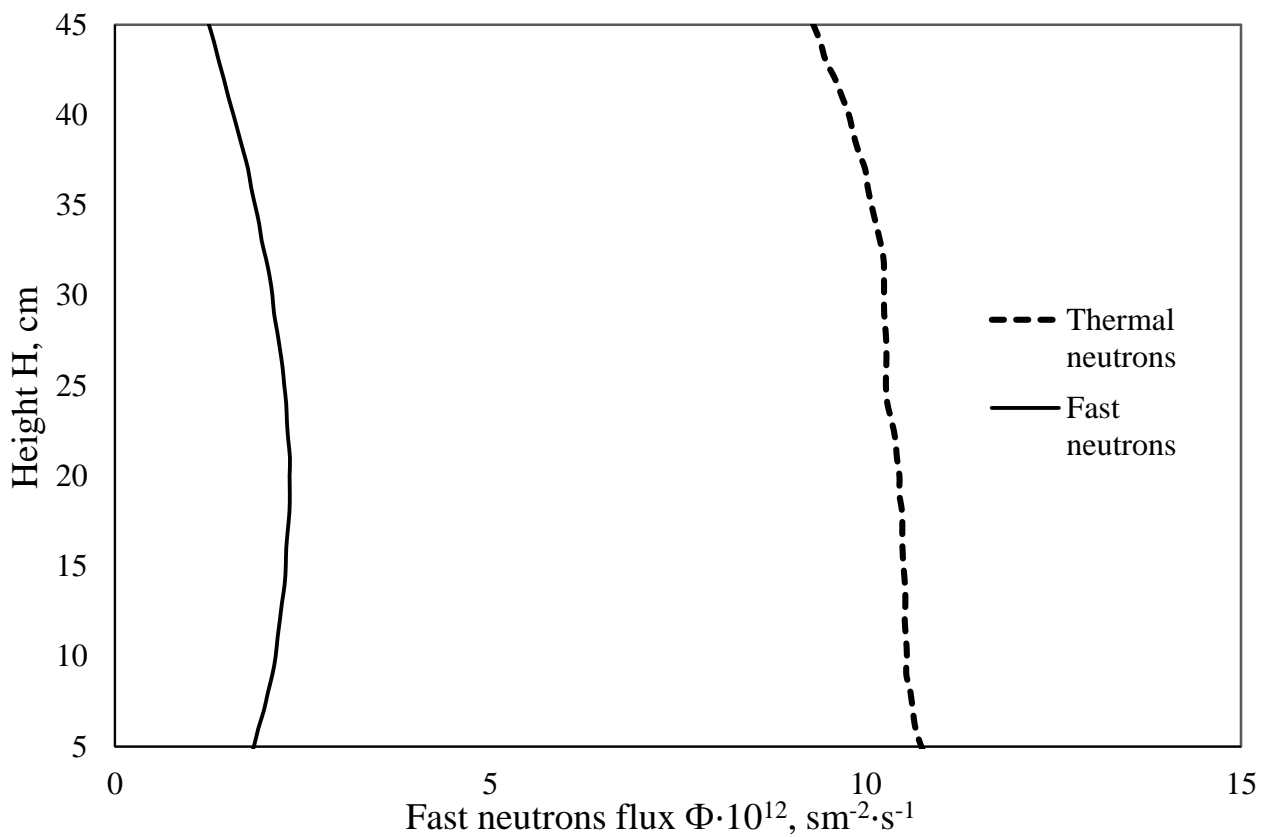


Figure 12 – Distribution of thermal neutron fluxes along the height of the container

It can be seen that without the use of absorbers, the average thermal neutron flux along the height of the container is  $\overline{\Phi_{th}} = 1.02 \cdot 10^{13} \text{ cm}^{-2} \cdot \text{s}^{-1}$ , the average fast neutron flux is  $\overline{\Phi_f} = 1.87 \cdot 10^{12} \text{ cm}^{-2} \cdot \text{s}^{-1}$ . The ratio of fast neutrons to thermal is  $k = \frac{\overline{\Phi_f}}{\overline{\Phi_{th}}} = 0.184$ , which is an unacceptable value for the use of an irradiating installation for irradiating

semiprecious stones. Thus, we can conclude that it is necessary to use a thermal neutron filter.

Consider the different configuration of the filters: we will use different filter materials and their different thicknesses. In each case, we calculate the average value of the flux of fast and thermal neutrons and the ratio of the average flux of fast neutrons to thermal. We will carry out a comparative characteristic of the absorbers used and determine the optimal operating conditions of the designed installation.

### 3.2 Applying of thermal neutron filters

As a thermal neutron filter, substances that actively absorb thermal neutrons, such as boron carbide, cadmium, hafnium, etc., can be used. In the course of the calculations, the average values of the fluxes of fast and thermal neutrons in the container are obtained. At first, an absorber made in the form of a cylindrical wall without end absorbing inserts is considered, as shown in Figure 13a.

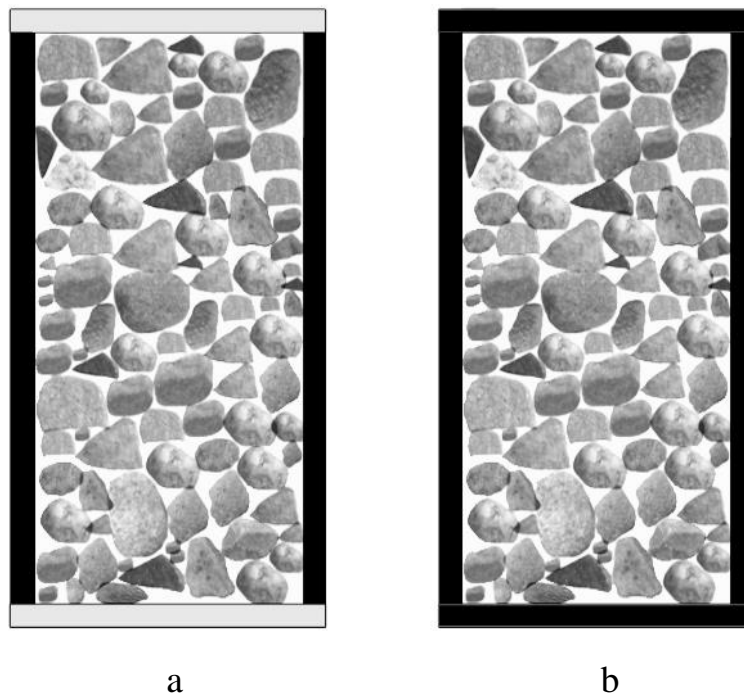


Figure 13 – Schematic representation of container for irradiation with thermal neutrons filter: a) with radial absorber; b) with radial and axial end absorber

The values were obtained for two thermal neutron absorbers - cadmium with density  $\rho = 8.65 \text{ g/cm}^3$  and boron carbide with density  $\rho = 2.34 \text{ g/cm}^3$  and for container without absorbing filter (with aluminum walls instead of boron carbide). Different

thicknesses of absorbers equal to 1, 2, and 3 mm are considered. The results of the calculation are presented in Table 2. In addition, the value of the ratio of the fast neutron flux to thermal  $k = \frac{\overline{\Phi}_f}{\overline{\Phi}_{th}}$ , the values of which are also presented in Table 2.

Table 2 – Calculation results

	Al	Cd ( $\delta = 1$ mm)	Cd ( $\delta = 2$ mm)	Cd ( $\delta = 3$ mm)	B <sub>4</sub> C ( $\delta = 1$ mm)	B <sub>4</sub> C ( $\delta = 2$ mm)	B <sub>4</sub> C ( $\delta = 3$ mm)
$\overline{\Phi}_{th} \cdot 10^{12},$ cm <sup>-2</sup> ·s <sup>-1</sup>	10.171	0.838	0.745	0.688	0.305	0.267	0.249
$\overline{\Phi}_f \cdot 10^{12},$ cm <sup>-2</sup> ·s <sup>-1</sup>	1.874	1.201	1.193	1.186	1.140	1.141	1.179
$k$	0.184	1.434	1.601	1.725	3.737	4.276	4.734

An analysis of the calculations shows that the use of filters significantly weakens the flow of thermal neutrons. The highest influence is exerted by boron carbide used. Let us analyze the values of the coefficient of the ratio of fast neutrons to thermal: it is clear that the use of boron carbide has an advantage over the use of cadmium with the same filter wall thickness. At the same time, we can see that a further increase in the wall thickness of the container does not make much sense, because the value of the thermal neutron flux with a further increase in thickness decreases slightly. Moreover, the ratio of the fast neutron flux to thermal in the container is unacceptable for the implementation of the technology for irradiating semiprecious stones.

However, considering the distribution of thermal neutrons along the height of the container, shown in Figure 14, it can be seen that there is a sharp increase in the thermal neutron flux at the ends of the container, which makes a significant contribution to the average flux.

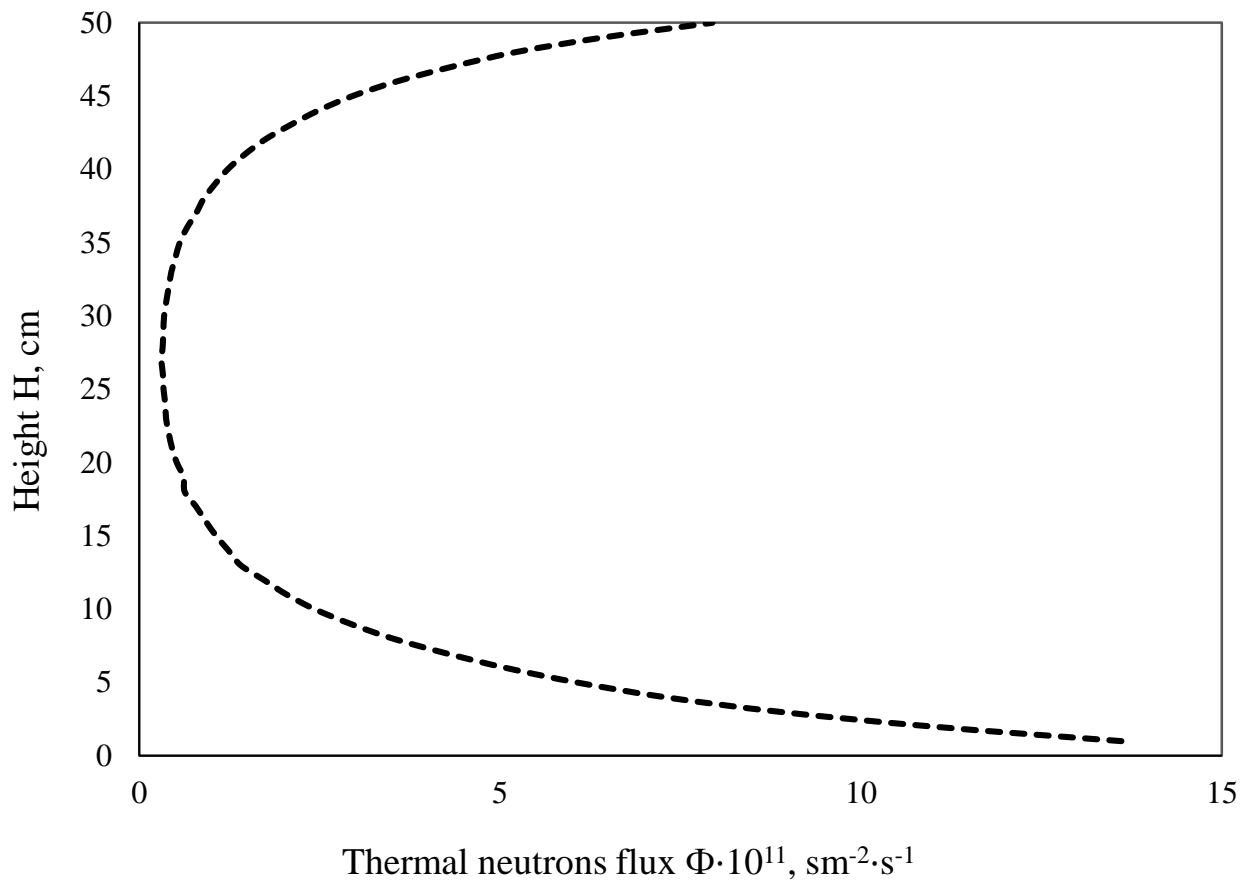


Figure 14 – Thermal neutron flux distribution over the height of the container

A sharp increase in the thermal neutrons flux at the ends of the container is due to the neutron reflective properties of the water in the channel in which the container is located. Thus, it is necessary to use an end absorber made of a material absorbing thermal neutrons. In the future, it is customary to use boron carbide in the calculations. Add end absorber with thickness of 3 mm to the existing model as shown in Figure 13b. The distribution of the thermal neutron flux along the height of the container before and after using the neutron absorber is shown in Figure 15.

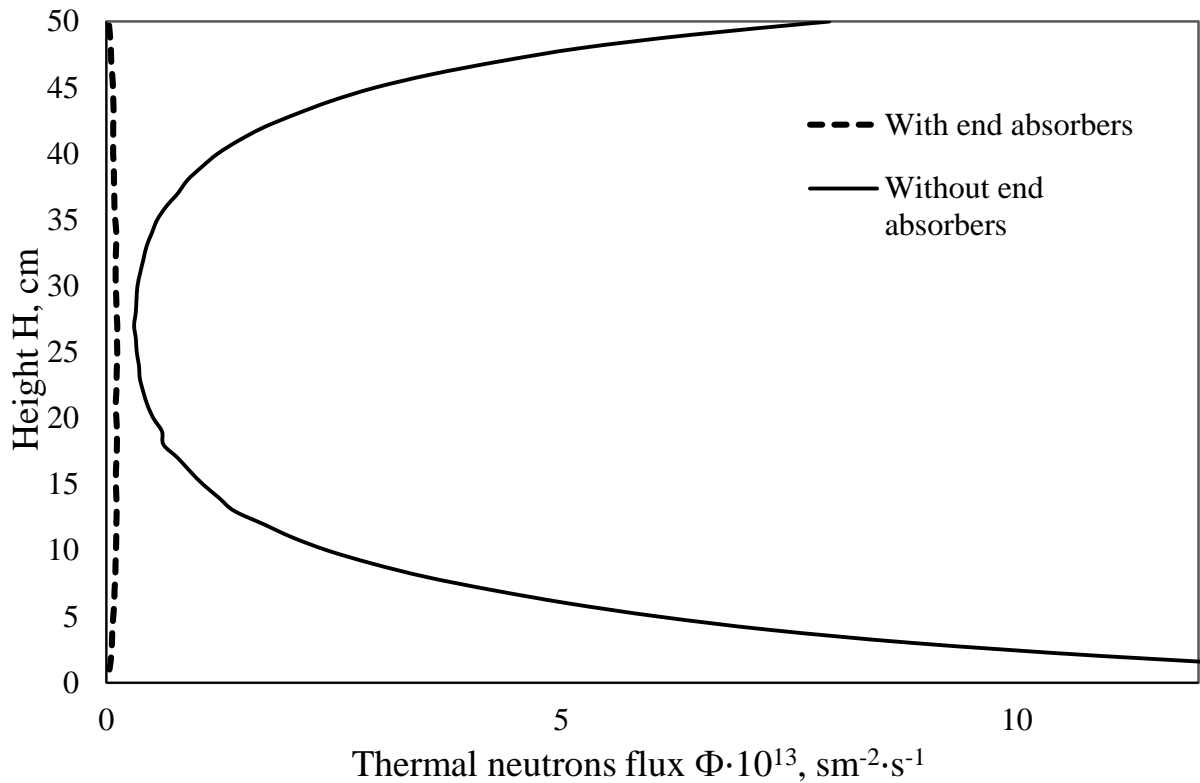


Figure 15 – Thermal neutron flux distribution with end absorbers

Here we can see how the redistribution of the thermal neutron flux occurs and the average value of the thermal neutron flux decreases along the height of the container when using end absorbers. The value of the thermal neutron flux is  $\overline{\Phi}_{th} = 9.09 \cdot 10^9 \text{ cm}^{-2}\text{s}^{-1}$ , the average fast neutron flux is  $\overline{\Phi}_f = 1.139 \cdot 10^{12} \text{ cm}^{-2}\text{s}^{-1}$ . The ratio of fast neutrons to thermal is  $k = \frac{\overline{\Phi}_f}{\overline{\Phi}_{th}} = 125.286$ , which meets the necessary requirements.

Thus, we can conclude that the topaz irradiation technology can be implemented in the experimental channel being designed: to create the necessary working conditions, the use of an absorbing filter made of boron carbide with a density  $\rho = 2.34 \text{ g/cm}^3$  is chosen, while the thickness is 3 mm.

The next step is to calculate the temperature conditions in the container. The energy release is calculated for different container radii and the maximum temperatures in the container and their correspondence to the permissible temperature during irradiation are determined.

## 4 Thermohydraulic calculation of a container with topazes

To determine the maximum temperature in the container with topazes, the specific energy release in the container was calculated in the MCU software. In this case, the radius of the container changed, and for each case, the energy release value  $q_v$  is determined: in irradiated topazes  $q_1$  and in the filter container  $q_2$ , as well as the total heat flux emitted from the boundaries of the container.

At the same time, it was taken into account that neutrons and gamma rays contributed to the energy release:

$$q_v = q_v^n + q_v^\gamma \quad (1)$$

The calculated energy release values are presented in Table 3.

Table 3 – Energy release in the container

$R_1$ , cm	$Q_1$ , kW	$Q_2$ , kW	$q_1$ , W/cm <sup>3</sup>	$q_2$ , W/cm <sup>3</sup>	$q_v$ , W/cm <sup>3</sup>
10.2	3.27	2.54	0.208	2.654	0.349
9.2	2.67	1.90	0.210	2.200	0.336
8.2	2.19	1.55	0.218	2.012	0.345
7.2	1.60	1.16	0.208	1.720	0.329
6.2	1.20	0.89	0.213	1.537	0.336
5.2	0.85	0.67	0.215	1.385	0.344

It can be noted that the results obtained are consistent with other studies where, in [26], in a prismatic container with dimensions of 6.5x6.5x80 cm, the energy release amounted to 0.18 W/cm<sup>3</sup>, in [1], in a cylindrical container with an internal useful radius of 4 cm and a height of 55 cm, the energy release was 0.265 W/cm<sup>3</sup>. The next step is to analyze the temperature distribution along the radius of the irradiated container and its dependence on the calculated energy release.

### 4.1 Radial temperature distribution in the container

In the general case, the temperature on the outer wall of the container is related to the energy release by Newton-Richmann law:



$$Q = F \cdot \alpha \cdot (t_w - t_l) \quad (2)$$

where  $Q = \pi \cdot R^2 \cdot H \cdot q_v$  – heat flux, W.

$\alpha$  – heat transfer coefficient,  $W/m^2K$ ;

$t_l$  – temperature of water, °C;

$t_w$  – temperature of outer wall, °C

$F$  – heat exchange surface area,  $m^2$

To determine the temperature in the center of the container, consider the temperature distribution along the radius of the container. Consider a model of a vertical rod without insulation, with an internal heat source, which will be equivalent to topaz irradiated without a container. A diagram of such a calculation model for thermohydraulic calculation is shown in Figure 16a. Heat is removed through the outer surface to the water along the radius  $r$ .

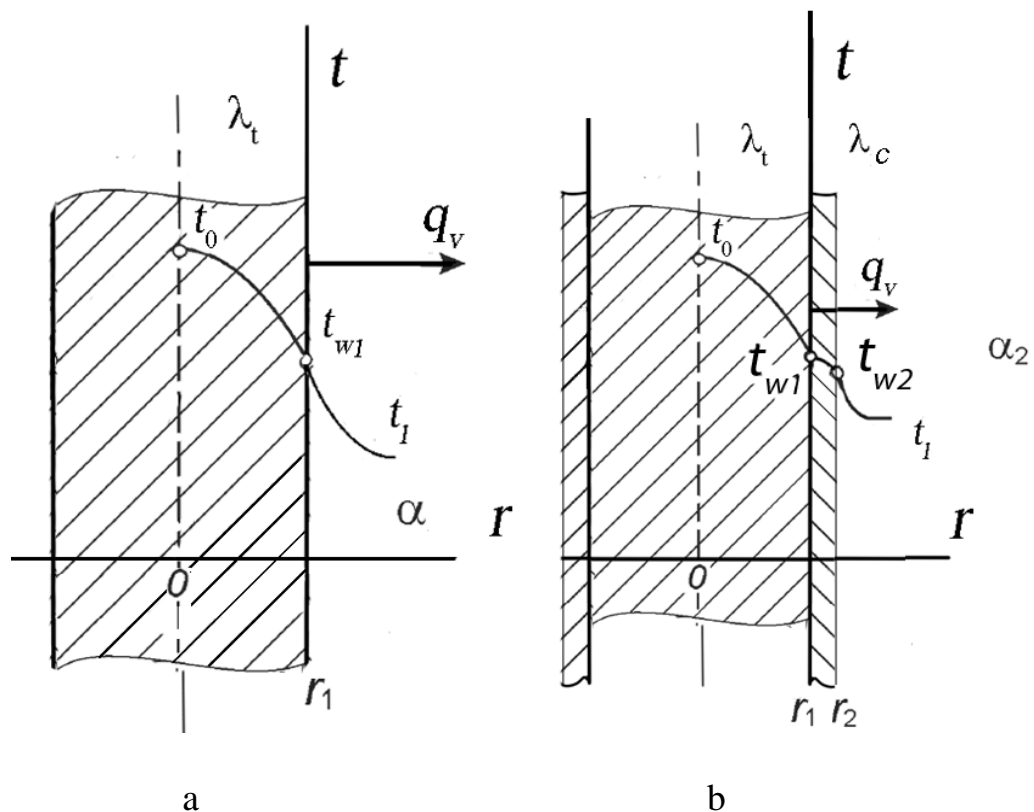


Figure 16 – Thermohydraulic Calculation Model scheme: a) bare rod with internal heat source; b) rod with insulation with internal heat source

When solving the differential heat equation [27] for this case, the temperature distribution along the radius of the bare rod is determined:

$$t(r) = t_l + \frac{q_v \cdot R_1}{2 \cdot \alpha} + \frac{q_v}{4 \cdot \lambda_t} \cdot (R_1^2 - r^2) \quad (3)$$

Then temperature on the axis of the rod:

$$t_0 = t_l + \frac{q_v \cdot R_1}{2 \cdot \alpha} + \frac{q_v \cdot R_1^2}{4 \cdot \lambda_t}$$

And temperature of the wall:

$$t_w = t_l + \frac{q_v \cdot R_1}{2 \cdot \alpha}$$

So we can conclude that

$$t_0 = t_w + \frac{q_v \cdot R_1^2}{4 \cdot \lambda_t}$$

Thus we can say that the temperature in the center of the container depends only on the thermal conductivity of the topaz and the temperature of the outer wall of the topaz, and does not depend on the thickness and material of the insulation

Consider Figure 16b, which designates a cylindrical rod with an internal heat source coated with insulation. In our case, this scheme is equivalent to a container with a thickness  $\delta = r_2 - r_1$  inside which topazes are poured. For this case, the solution of the differential equation of heat transfer gives the following equation:

$$Q = \pi \cdot R_1^2 \cdot H \cdot q_v = \frac{t_{w1} - t_l}{\frac{1}{2\pi \cdot H \cdot \lambda_c} \ln\left(\frac{R_2}{R_1}\right) + \frac{1}{2\pi \cdot H \cdot \alpha_2 \cdot R_2}}, \quad (4)$$

And we obtain:

$$t_{w1} = t_l + \frac{q_v \cdot R_1^2}{2 \cdot \lambda_c} \ln\left(\frac{R_2}{R_1}\right) + \frac{q_v \cdot R_1^2}{\alpha_2 \cdot R_2} \quad (5)$$

Here the temperature in the center will be determined as:

$$t_0 = t_{w1} + \frac{q_v \cdot R_1^2}{4 \cdot \lambda_t} = t_{w1} + \frac{q_v \cdot R_1^2}{4 \cdot \lambda_{eff}} \quad (6)$$

Here, the average effective thermal conductivity is calculated according to the law of the average value of the function in the interval:

$$\overline{\lambda_{eff}} = \frac{1}{t_0 - t_{w1}} \cdot \int_{t_{w1}}^{t_0} \lambda_{eff}(t) dt = \frac{1}{t_0 - t_{w1}} \cdot \int_{t_{w1}}^{t_0} (0.004673 \cdot t + 0.647166) dt$$

So the main task is to determine the heat transfer coefficient from the outer wall of the container to the water  $\alpha_2$ .

#### 4.2 Determining the heat transfer coefficient

In general, the heat transfer coefficient can be written as:

$$\alpha_2 = \alpha = \frac{Nu_l \cdot \lambda_l}{H} \quad (7)$$

The Nusselt number:

$$Nu_l = 0,76 (Gr_l \cdot Pr_l)^{0,25} \cdot \left( \frac{Pr_l}{Pr_{w2}} \right)^{0,25}$$

The Grashof number:

$$Gr_l = \frac{\beta \cdot g \cdot H^3 \cdot (t_{w2} - t_l)}{\nu_l^2}$$

Finally, for the heat transfer coefficient we have:

$$\alpha = 0,76 \left( \frac{\beta \cdot g \cdot H^3 \cdot (t_{w2} - t_l)}{\nu_l^2} \cdot Pr_l \right)^{0,25} \cdot \left( \frac{Pr_l}{Pr_{w2}} \right)^{0,25} \cdot \frac{\lambda_l}{H}$$

Using the Newton-Richmann law for our case we obtain:

$$q_v = \frac{2}{R_2} \cdot 0,76 \cdot \left( \frac{\beta \cdot g \cdot H^3 \cdot (t_{w2} - t_l)}{\nu_l^2} \cdot Pr_l \right)^{0,25} \cdot \left( \frac{Pr_l}{Pr_{w2}} \right)^{0,25} \cdot \frac{\lambda_l}{H} \cdot (t_{w2} - t_l)$$

$$2 \cdot 0,76 \cdot \left( \frac{\beta \cdot g \cdot H^3}{\nu_l^2} \right)^{0,25} \cdot \frac{\lambda_l}{H} \cdot \sqrt{Pr_l} \cdot (t_{w2} - t_l)^{1,25} = q_v \cdot (Pr_{w2})^{0,25} \cdot R_2$$

The calculation data are taken for the liquid pressure in the channel  $p_l = 68.67$  kPa (for a height of 7 m), water temperature  $t_l = 40$  °C. At this temperature and pressure: thermal conductivity of water  $\lambda_l = 0.623$  W/mK, kinematic viscosity

coefficient  $\nu = 6.959 \cdot 10^{-7} \text{ m}^2/\text{s}$ , thermal expansion coefficient  $\beta = 3.226 \cdot 10^{-3} \text{ K}^{-1}$ , Prandtl number for water  $Pr_l = 4.6258$ .

Using the known values, we finally obtain the equation:

$$1227.91 \cdot (t_{w2} - 40)^{1,25} = q_v \cdot (Pr_{w2})^{0,25} \cdot R_2 \quad (8)$$

The resulting expression (8) is an equation for the desired outer wall temperature. Solving this equation, we obtain the temperature values of the outer wall, then using the formula (7) we determine the value of heat transfer coefficient. Summarize all the calculated values in Table 4.

Table 4 – Calculation of heat transfer coefficient

$R_l, \text{ cm}$	$q_v, \text{ W/cm}^3$	$t_{w2}, \text{ }^\circ\text{C}$	$\alpha, \text{ W/m}^2\text{K}$
10.2	0.349	58.53	960.17
9.2	0.336	56.66	927.78
8.2	0.345	55.57	907.98
7.2	0.329	53.61	871.42
6.2	0.336	52.33	843.67
5.2	0.344	50.97	815.10

Next, for the radius values, using the calculated values of the heat transfer coefficient by the formula (5), we determine the temperature at the topaz and container boundaries  $t_{w1}$  and then by the formula (6) the desired temperature in the center of the container  $t_0$ .

It should be taken into account the value of thermal conductivity of boron carbide which is used as the material of the container. Studies [28-29] show that in the range of operating temperatures the thermal conductivity of boron carbide  $\lambda_{B_4C}$  (both for compound  $^{10}\text{B}_4\text{C}$ , and for  $^{11}\text{B}_4\text{C}$ ) slightly varies within 25-30 W/mK. For calculations, we take the value  $\lambda_{B_4C} = 27 \text{ W/mK}$ . The calculation results are listed in Table 5.

Table 5 – Calculation of the maximal temperature

$R_1$ , cm	$q_1$ , W/cm <sup>3</sup>	$t_{w1}$ , °C	$t_0$ , °C
10.2	0.208	73.61	342.230
9.2	0.210	69.64	301.315
8.2	0.218	67.25	266.215
7.2	0.208	63.10	218.646
6.2	0.213	60.30	183.462
5.2	0.215	57.30	146.456

Thus, we can conclude that it is necessary to reduce the useful radius of the container. However, to clarify the result, it is necessary to carry out software simulation of the model and compare the results obtained by hand calculation with the results of computer modeling, and draw a conclusion about the value by which the radius of the container should be reduced to comply with the required temperature conditions. After this, it is required to evaluate the induced activity of topazes when they are irradiated in the container.

#### 4.3 Software calculation

To confirm the calculated data, we use the universal software platform for modeling physical processes COMSOL Multiphysics®. The first step is to create the geometry, the model shown in Figure 17.

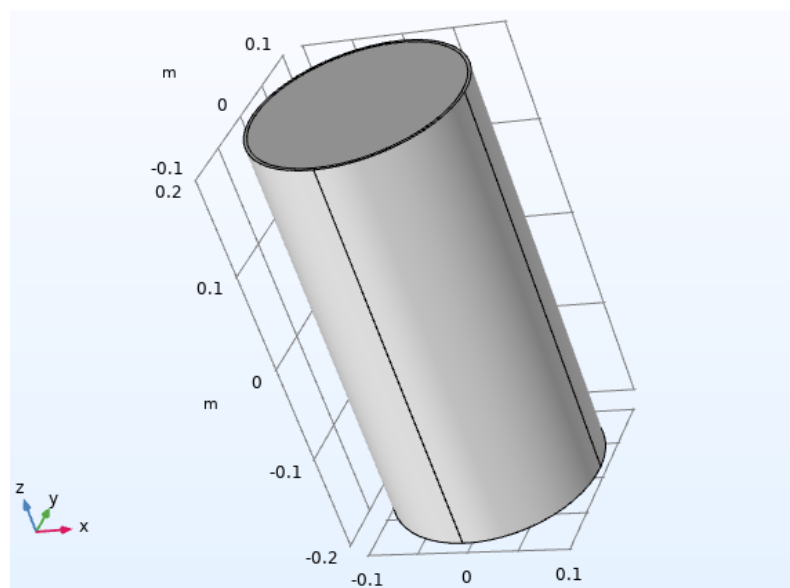


Figure 17 – Geometry of the calculation model

The geometry is a vertically oriented cylinder imitating a container for irradiation, inside which a useful volume for irradiating topazes is coaxially located. This is shown in more detail in Figure 18.

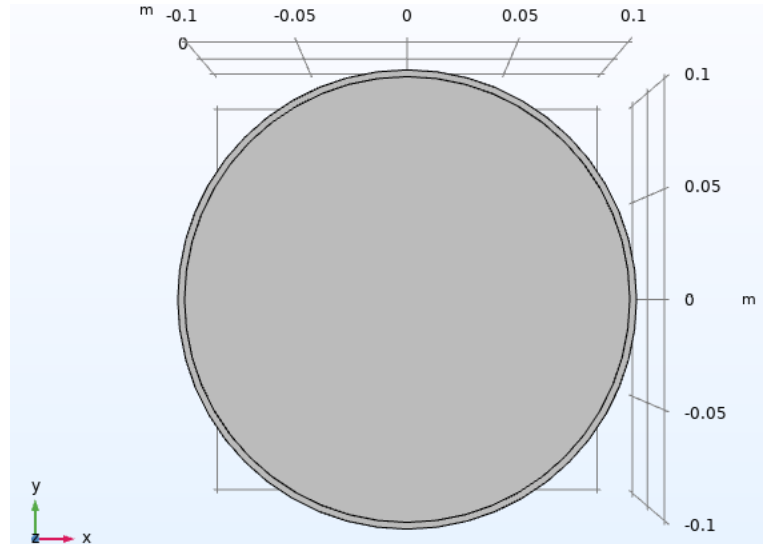


Figure 18 – Lengthwise cross-section of container

COMSOL Multiphysics® software platform has a special physical module **Heat Transfer in Porous Media**, allowing the calculation of porous systems. In the general case, the module consists of physical media, such as solids, fluids and porous systems, heat sources (volumetric and boundary) and heat fluxes, and the geometry associated with the module. Applicable to the case considered in this paper, the interface will consist of the components shown in Figure 19.

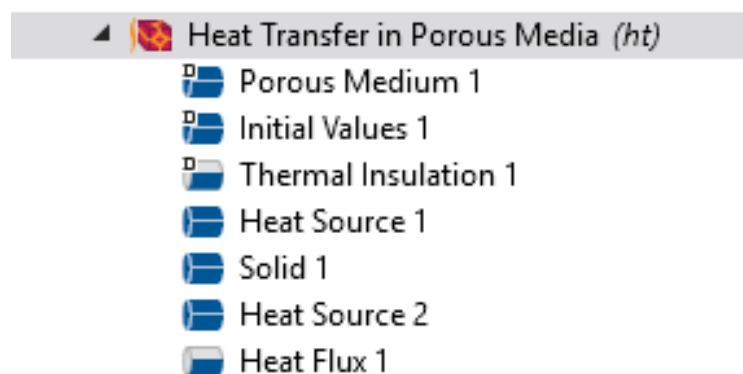


Figure 19 – Composition of Heat Transfer in Porous Media module

Here, the main component of the module is *Porous Medium 1*, a component that describes a porous medium itself. In this case, topaz bulk. For the calculation, the

volume fraction of the solid phase is equivalent to  $(1-m)$  is used, the thermal conductivities of the solid and fluid phases (in this case, air) and other physical quantities are needed for the calculations. The *Solid 1* component describes a solid carbide container made of boron carbide. For the calculation, the values of thermal conductivity, density, and other physical constants for the material are set. The components *Heat Source 1* and *Heat Source 2* describe the sources of energy release and their power, which is set from the previously calculated values of  $Q_1$  and  $Q_2$ , in watts, for energy release from the volume of topazes and from the volume of the walls of the container, respectively. The *Heat Flux 1* component describes convective heat transfer from a container with topazes to water: the temperature and pressure of the water, the height of the cylindrical container, its diameter and the boundaries of heat transfer are set. The *Thermal Insulation 1* component is optional, the boundaries through which heat exchange does not occur are set, the initial temperature in the container, accepted  $20\text{ }^\circ\text{C}$ , is set in the *Initial Values 1* component.

The calculation of the constructed model is performed. Figures 20-21 show the temperature distribution over the surface of the container.

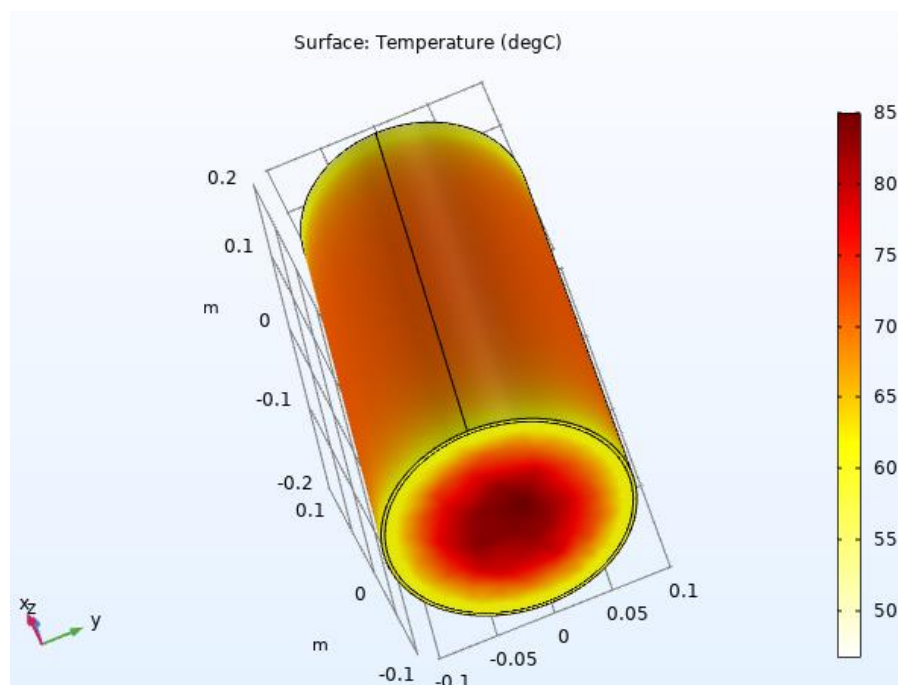


Figure 20 – Bottom view

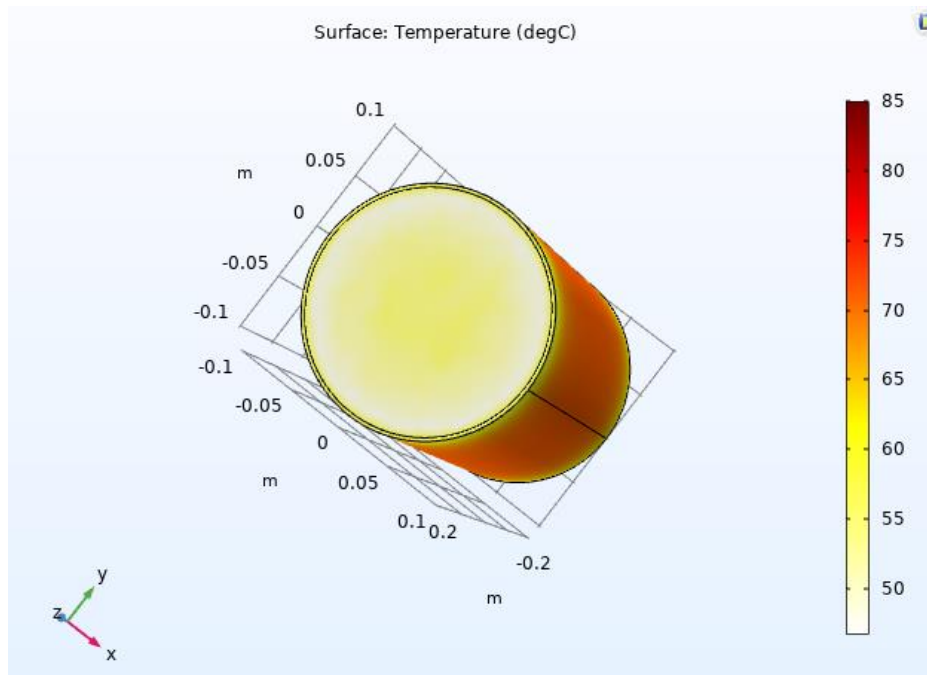


Figure 21 – View from above

Figures 22-23 show the radial temperature distribution in the container for different container radii.

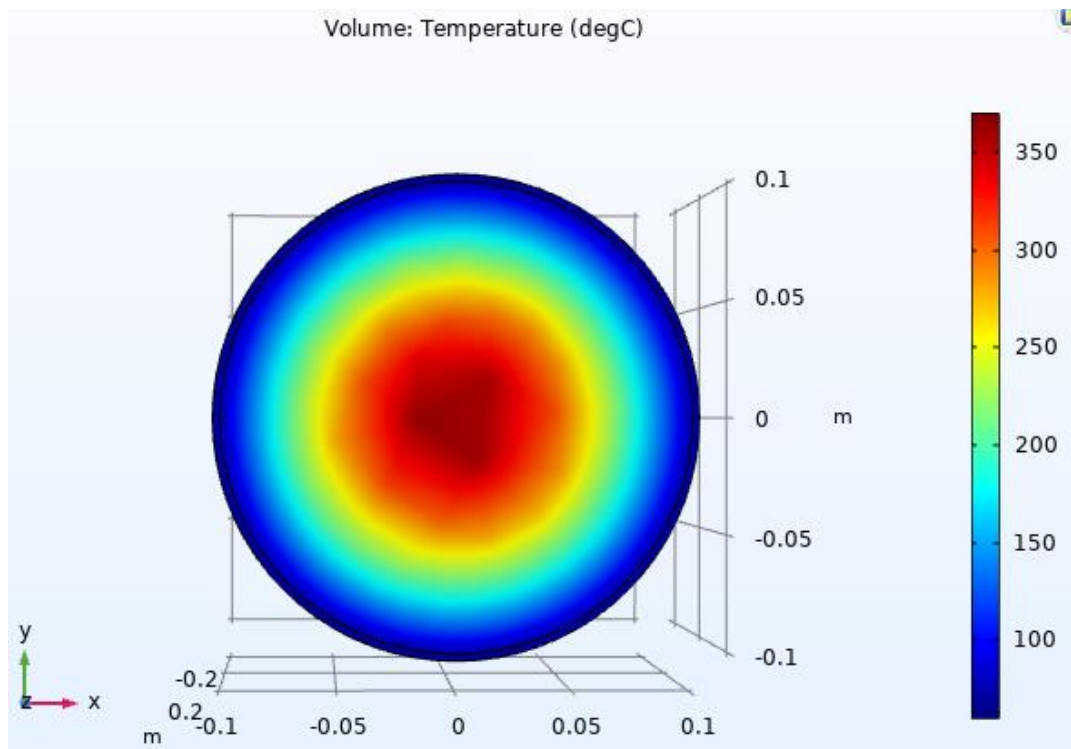


Figure 22 – Radial temperature distribution in the container ( $R_2 = 10.2$  cm)



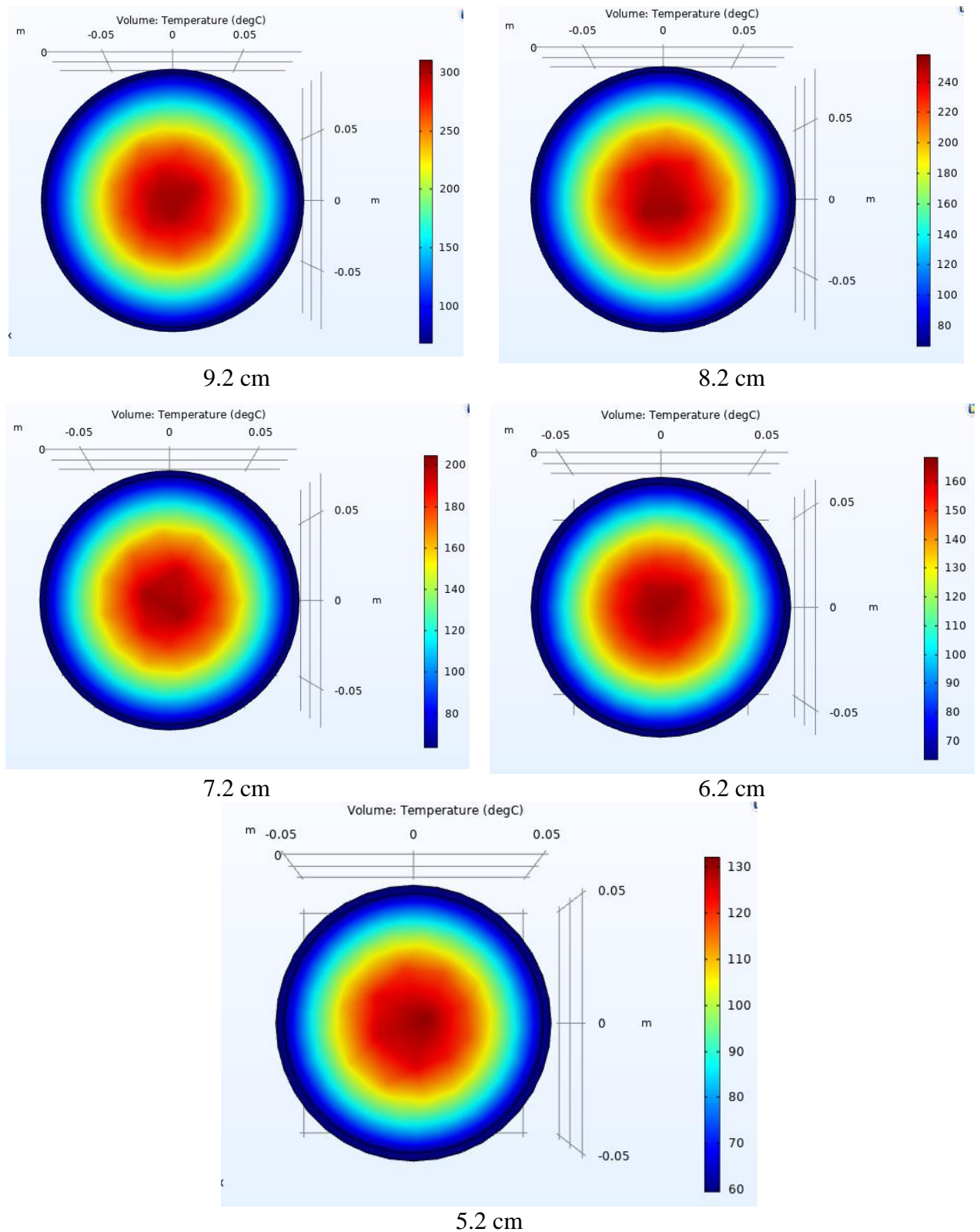


Figure 23 – Radial temperature distribution in the container for other  $R_2$

Thus, from Figures 20 and 21 it can be seen that when the container is cooled due to natural convection in the water, the end faces of the container are cooled, while the upper face cools better than the lower one. From the data of Figures 22-23, it was concluded that when the radius of the container decreases, the maximum temperature

in the center also decreases. Table 6 shows comparisons of the maximum temperature values calculated in the COMSOL program and in theoretical calculation of  $t_0, ^\circ\text{C}$ .

Table 6 – Comparison of the maximum temperature in container

$R_{\text{eff}}, \text{cm}$	$t_0, ^\circ\text{C}$ (COMSOL)	$t_0, ^\circ\text{C}$ (hand)	$\delta, \%$
9.9	370.931	342.230	-8.39
8.9	310.756	301.315	-3.04
7.9	258.1402	266.215	3.13
6.9	204.825	218.646	6.75
5.9	168.531	183.462	8.86
4.9	132.257	146.456	10.74

In Figure 24 we can see the dependence of the temperature in the center of the container on the radius of the container.

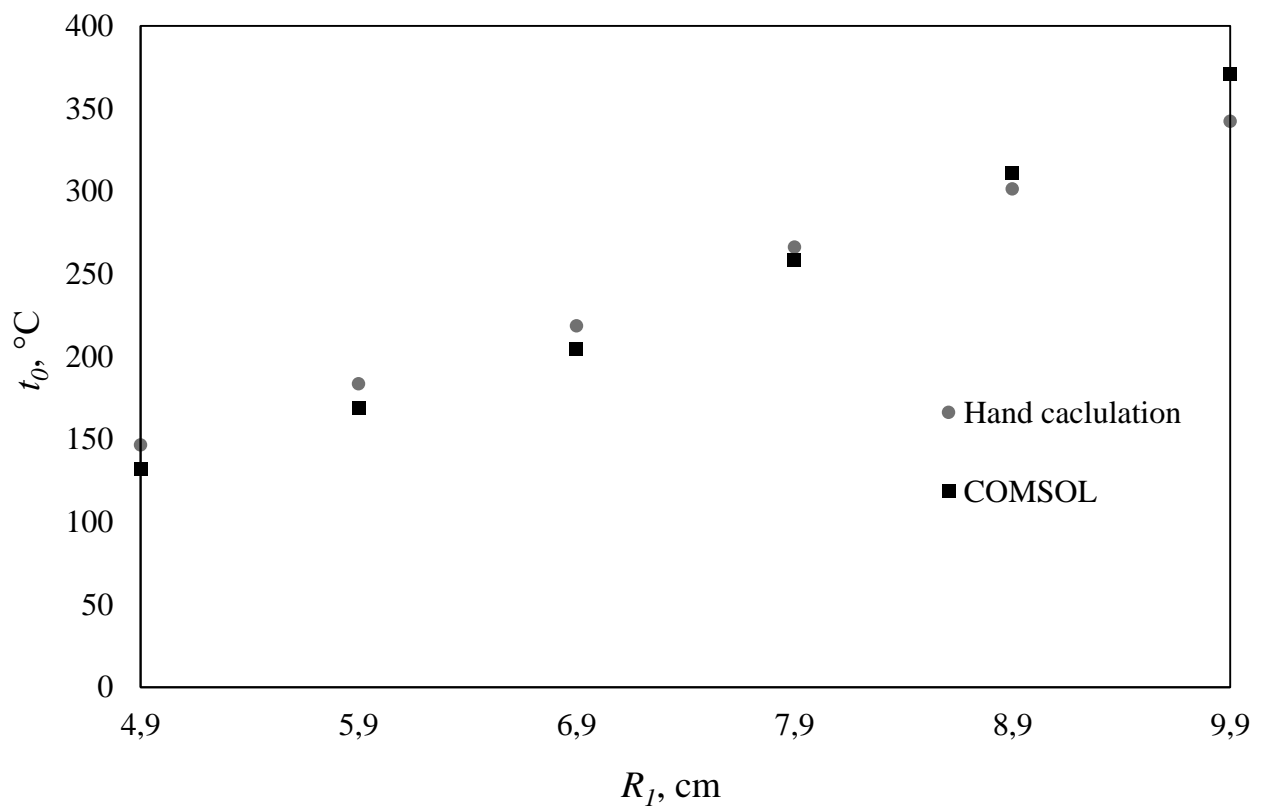


Figure 24 – The dependence of the temperature in the center of the container on the radius

We can check the use of a theoretical apparatus for calculating the radial temperature distribution by specifying the porosity value  $m = 0$  in the model used in COMSOL. This means that the system will go into a non-porous state, and the effective thermal conductivity of the bulk will be equivalent to the thermal conductivity of topazes:  $\lambda_{eff} = \lambda_s$ . The obtained temperature distribution for the outer radius of the container  $R_2 = 10.2$  cm presented in Figure 25.

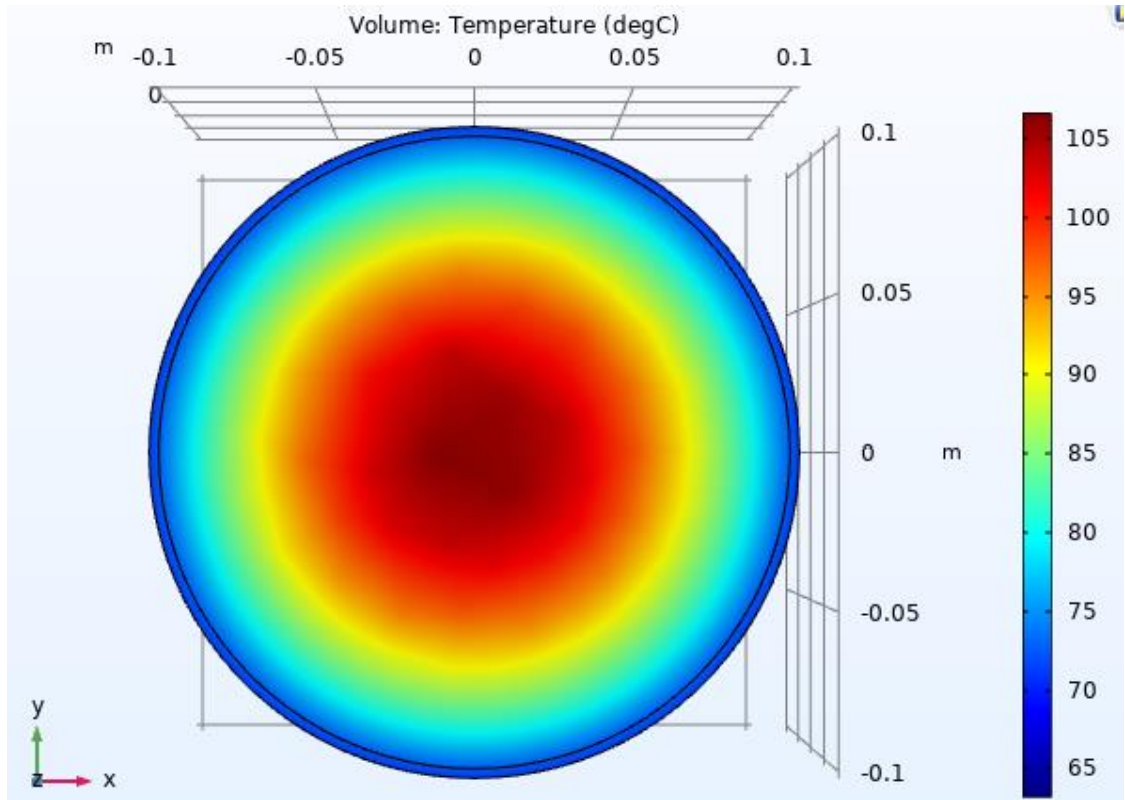


Figure 25 – Radial temperature distribution in non-porous state

In addition, the temperature value in the center of the container was calculated using theoretical formulas. Table 7 shows the maximum temperatures for theoretical calculation and for calculation in the COMSOL program.

Table 7 – Comparison of the maximum temperature in non-porous state

$R_2$ , cm	$t_0$ , °C (hand)	$t_0$ , °C (COMSOL)	$\delta$ , %
10.2	102.694	106.040	3.16

As can be seen from the data obtained, in the transition to a non-porous system, the difference in theoretical and software calculations is minimal. It can be concluded that the main contribution to the calculation error is made by the value of effective thermal conductivity: the formulas used to calculate the effective thermal conductivity are approximate and do not take into account many factors of real porous systems, based only on geometric approximations, such as the transition from random filling of particles of different sizes to spherical filling, as well as the impossibility of real measurement of pore size in particles.

Based on the foregoing, guided by the calculation of the COMSOL software package, we can conclude that the permissible radius of the container during irradiation is the value of the internal radius  $R_7=6.9$  cm. The next step in the study is to calculate the induced activity upon irradiation of topazes in the reactor channel.

## 5 Calculation of induced activity in irradiated samples

The next step in the study considered in this paper is the calculation of the induced activity in the irradiated samples. It is necessary to analyze the impurities found in natural topazes before they are irradiated with a neutron flux, which after irradiation are a source of radioactive nuclides that contribute to the induced activity of topazes; it is also necessary to estimate the magnitude of the induced radioactivity in topazes and compare its value with regulated norms, and also if the induced activity exceeds the permissible level, it is necessary to calculate the delay time of the irradiated samples before use by their consumers.

### 5.1 Calculation of operating conditions for a new container radius

Before calculating the activity in the samples, it is necessary to make sure that the selected radius of the container ensures compliance with the conditions for the ratio of the flux of fast neutrons to thermal, discussed in the second chapter of this paper.

Figure 26 shows the distribution of fast and thermal neutron fluxes for an outer radius of the container of 7.2 mm over the height of the container.

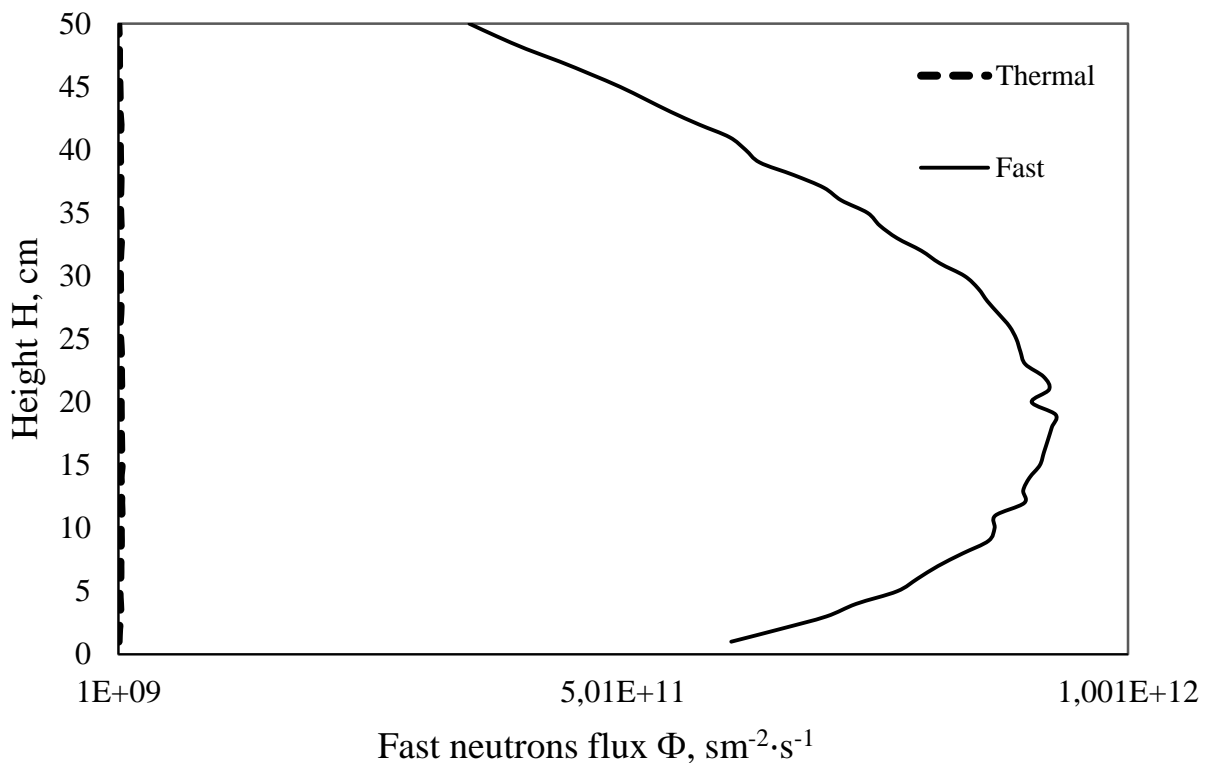


Figure 26 – Thermal neutron flux distribution for  $R_2 = 7.2$  cm

It is seen that a decrease in the radius of the container with topaz leads to an increase in the fraction of water in the experimental channel, which leads to an increase in the absorption of thermal neutrons. In this case, the ratio of fast to thermal neutrons was  $k = 273.96$ , which satisfies the necessary condition. The value of the average fast neutron flux is  $7.52 \cdot 10^{11} \text{ n/cm}^2\text{s}$ .

Now we determine what impurities are contained in unirradiated topazes and calculate the induced activity after irradiation.

## **5.2 Calculation of induced activity**

The next step is to evaluate the induced activity in the container after irradiation. It is known that to achieve the necessary results of irradiation, it is necessary to irradiate the container with fast neutrons of 1 MeV with fluence up to  $10^{17}$ - $10^{18} \text{ n/cm}^2$  [6, 22-25, 30], which subsequently provides different shades of blue topaz color, depending on the magnitude of the fluence. Increase in fluence over  $10^{18} \text{ cm}^{-2}$  impractical due to increased radioactivity of the processed minerals. According to the calculations made in the previous paragraph of this chapter of the study, the average fast neutron flux was  $7.52 \cdot 10^{11} \text{ n/cm}^2\text{s}$ . We take the value of the necessary fluence equal to  $F = 10^{17} \text{ n/cm}^2$ . Accordingly, the exposure time is determined from the ratio  $F = \Phi \cdot t$  and will be equal  $t = 1.33 \cdot 10^5 \text{ s}$ , which is equivalent to 1.54 days.

In the first chapter, when considering the chemical composition of topazes, it was mentioned that in addition to the main elements, the composition of stones also includes a number of impurity elements. When a container with topazes is irradiated, these elements form a significant part of the induced activity and can have a negative impact on the possibility of using irradiated stones by the consumer.

The presence of certain impurities, as well as their volume concentration, depends on the topaz deposit. Topaz samples from various deposits, such as Brazil and China, were considered [5–7]. Table 8 presents the most common impurity atoms found in topaz, the average fraction per million of topaz atoms, and calculated impurity concentrations.

Table 8 – Most common impurities in topaz samples

Nuclide	ppm	$N_i \cdot 10^{16}, \text{cm}^{-3}$
Ca <sup>44</sup>	481.63	366.677
Na <sup>23</sup>	240.15	182.831
Cr <sup>52</sup>	32.04	24.389
Ti <sup>47</sup>	26.43	20.124
B <sup>11</sup> ,	13.10	9.973
Fe <sup>56</sup>	6.05	4.606
K <sup>39</sup>	5.28	4.020
Li <sup>7</sup>	2.45	1.861
Mg <sup>24</sup>	2.14	1.629
Ga <sup>71</sup>	1.81	1.378
V <sup>51</sup>	1.71	1.300
Sc <sup>45</sup>	1.47	1.121
Cs <sup>133</sup>	0.10	0.079
Mn <sup>55</sup>	4.175	3.179
Cu <sup>63</sup>	3.955	3.011
Zn <sup>90</sup>	4.12	3.137
Nb <sup>93</sup>	2.22	1.690
Ta <sup>181</sup>	1.66	1.264

All impurity elements are stable. However, when irradiated with a neutron flux, they can transmute into other radioactive nuclides, which will make a significant contribution to the induced activity of topazes. Thus, using the MCU software package, these impurities are added to the existing container model and the reactor burnup time is set to 1.54 days.

Table 9 presents the results of the calculation of the model, showing the elements present in the irradiated samples after a given exposure time, and giving a significant contribution to the induced activity, as well as their concentrations and half-lives. Taking into account the volume occupied by the topazes in the container with an internal radius of 6.9 cm and a height of 50 cm, as well as their masses, the specific activity of impurities was calculated, and also listed in Table 9.

Table 9 – Radionuclides in irradiated samples

Nuclide	$N_{i,}, \text{cm}^{-3}$	$T_{1/2}$	$A_i, \text{Bq/g}$
Ta <sup>182</sup>	$1.06 \cdot 10^{10}$	114.43 days	316.29
Ca <sup>45</sup>	$3.63 \cdot 10^9$	162.67 days	76.36
Cs <sup>134</sup>	$4.67 \cdot 10^9$	2.07 years	21.21
Sc <sup>46</sup>	$2.57 \cdot 10^8$	83.76 days	10.50
Cs <sup>135</sup>	67.3	2.912 hours	$1.90 \cdot 10^{-3}$
Ar <sup>39</sup>	$4.55 \cdot 10^8$	269 years	$1.58 \cdot 10^{-2}$
Ni <sup>63</sup>	$7.60 \cdot 10^7$	100.1 years	$7.11 \cdot 10^{-3}$
Ta <sup>183</sup>	$9.54 \cdot 10^3$	5.1 days	$6.40 \cdot 10^{-3}$
Mn <sup>54</sup>	$4.07 \cdot 10^5$	312.03 days	$4.46 \cdot 10^{-3}$
Co <sup>60</sup>	$1.44 \cdot 10^6$	5.27 years	$2.56 \cdot 10^{-3}$
Nb <sup>95</sup>	$2.23 \cdot 10^2$	34.99 days	$2.18 \cdot 10^{-5}$

It is seen that, after irradiation, the most significant contribution to the induced radioactivity is the presence of such elements as Ta<sup>182</sup>, Ca<sup>45</sup>, Sc<sup>46</sup>, which are active  $\beta^-$  emitters with a short half-life, and  $\beta^-$  emitter Cs<sup>134</sup>. It is known that the activity of each element in the samples contributes to the total activity. Thus, the activity of all elements in the container will be equivalent to the sum of the activities of the individual elements:  $A_i$  :

$$A = \sum A_i = A_1 + A_2 + \dots A_n .$$

After irradiation, the stones required to be set aside, in order to reduce the level of radioactivity. Each isotope decays according to the law of radioactive decay:

$$A(t) = A_1(t) + A_2(t) + \dots A_n(t) = A_{01} \cdot e^{-\lambda_1 t} + A_{02} \cdot e^{-\lambda_2 t} + \dots A_{0n} \cdot e^{-\lambda_n t} ,$$

Where:  $\lambda_i$  – decay constant of the  $i$ -th element,  $\text{s}^{-1}$ ;

$t$  – passed time, s.

According to [10,22-24,31], the maximum allowable level of specific activity established by the IAEA, above which it is forbidden to use irradiated stones by consumers, is  $\leq 74 \text{ Bq/g}$ . Let us take the time elapsed since the irradiated stones are set aside equal to  $t_i$ . We calculate the specific activity of topazes over time and determine the delay time  $t_d$ , is the time during which the induced activity of the irradiated samples



reaches an acceptable level. Table 10 presents the calculated values of the activity of individual nuclides, as well as the total specific activity of topazes in the container.

Table 10 – Specific activity of topazes

Nuclide	$\lambda, s^{-1}$	$A_i, \text{Bq/g}$						
		t = 0 days	t = 10 days	t = 50 days	t = 100 days	t = 200 days	t = 300 days	t = 342 days
Ta <sup>182</sup>	$7.01 \cdot 10^{-8}$	316.29	297.70	233.64	172.59	94.18	51.39	39.85
Ca <sup>45</sup>	$4.93 \cdot 10^{-8}$	76.36	73.18	61.71	49.87	32.57	21.27	17.78
Cs <sup>134</sup>	$1.06 \cdot 10^{-8}$	21.21	21.02	20.26	19.35	17.65	16.10	15.49
Sc <sup>46</sup>	$9.58 \cdot 10^{-8}$	10.50	9.66	6.94	4.59	2.01	0.88	0.62
Cs <sup>135</sup>	$6.61 \cdot 10^{-5}$	$1.90 \cdot 10^{-3}$	0.00	0.00	0.00	0.00	0.00	0.00
Ar <sup>39</sup>	$8.17 \cdot 10^{-11}$	$1.58 \cdot 10^{-2}$	$1.58 \cdot 10^{-2}$	$1.58 \cdot 10^{-2}$	$1.58 \cdot 10^{-2}$	$1.58 \cdot 10^{-2}$	$1.58 \cdot 10^{-2}$	$1.58 \cdot 10^{-2}$
Ni <sup>63</sup>	$2.20 \cdot 10^{-10}$	$7.11 \cdot 10^{-3}$	$7.11 \cdot 10^{-3}$	$7.11 \cdot 10^{-3}$	$7.10 \cdot 10^{-3}$	$7.08 \cdot 10^{-3}$	$7.07 \cdot 10^{-3}$	$7.07 \cdot 10^{-3}$
Ta <sup>183</sup>	$1.57 \cdot 10^{-6}$	$6.40 \cdot 10^{-3}$	$1.64 \cdot 10^{-3}$	$7.16 \cdot 10^{-6}$	$8.01 \cdot 10^{-9}$	$1.0 \cdot 10^{-14}$	$1.26 \cdot 10^{-20}$	$4.17 \cdot 10^{-23}$
Mn <sup>54</sup>	$2.57 \cdot 10^{-8}$	$4.46 \cdot 10^{-3}$	$4.37 \cdot 10^{-3}$	$3.99 \cdot 10^{-3}$	$3.57 \cdot 10^{-3}$	$2.86 \cdot 10^{-3}$	$2.29 \cdot 10^{-3}$	$2.09 \cdot 10^{-3}$
Co <sup>60</sup>	$4.17 \cdot 10^{-9}$	$2.56 \cdot 10^{-3}$	$2.55 \cdot 10^{-3}$	$2.51 \cdot 10^{-3}$	$2.47 \cdot 10^{-3}$	$2.38 \cdot 10^{-3}$	$2.29 \cdot 10^{-3}$	$2.26 \cdot 10^{-3}$
Nb <sup>95</sup>	$2.29 \cdot 10^{-7}$	$2.18 \cdot 10^{-5}$	$1.79 \cdot 10^{-5}$	$8.11 \cdot 10^{-6}$	$3.01 \cdot 10^{-6}$	$4.15 \cdot 10^{-7}$	$5.73 \cdot 10^{-8}$	$2.49 \cdot 10^{-8}$
$A = \sum A_i, \text{Bq/g}$		424.39	401.58	322.58	246.42	146.42	89.66	73.76

The calculated value of the delay time at which the induced activity falls below the permitted level is  $t_d = 342$  days. It should be said that this value substantially depends on the semiprecious stones deposit due to the different concentration and type of impurity atoms in different deposits, as well as on the type of semiprecious stones. It should be noticed that the exposure time after irradiation also depends on the neutron fluence. With an increase in fluence, the concentration of radioactive elements in irradiated stones increases: despite the fact that with an increase in fluence, the shade of topazes is darker, and hence jewelry value, the delay time may be too high value (many years) [10], which negates the economic component of the project. Thus, the determination of the optimal value of fluence during irradiation is the task of optimizing the irradiation facility: it is necessary to determine such a value at which the economically viable value of the delay time of semiprecious stones is observed, as well as the necessary shade of the finished product.

### **5.3 The final configuration of the irradiation facility**

Finally, we can conclude about the following configuration of the installation when using it to irradiate semiprecious stones in it, using the example of topazes. The irradiation container is made of aluminum cylinder coated with a neutron absorber made of 3 mm thick boron carbide and 1 mm end absorbers, while the ratio of fast neutron flux to thermal flux was  $k = 273.96$ , which is a value corresponding to the requirements. The internal useful radius of the container is 6.9 cm; the height of the container is 50 cm. According to the calculated dimensions and data, a 3D model of the container for irradiation is constructed, the model of which is presented in Appendix A. The 3D model of the experimental channel in which the container is irradiated is presented in Appendix B.

After irradiation in a container for a time of 1.54 days, topazes are set aside for 342 days to achieve the required value of specific induced activity caused by the presence of radioactive impurities equal to 74 Bq/g.

We can compare the resulting configuration with other existing installations for the irradiation of semiprecious stones. So, on one of the experimental channels of the IRT-T reactor, this technology already exists [1]; Similar installations were also

implemented at the Egyptian research reactor ETRR-2 [26], where a prismatic container is used, and also at the Thai reactor TRR-1/M1, cylindrical containers are used [32]. Let us compare the useful volume for topaz irradiation, which is directly related to the productivity of the irradiating installation, for the other reactors under consideration. The resulting comparison is presented in Table 11.

Table 11 – Comparison of existing facilities

Reactor	Type of irradiation container	Dimensions	Volume, cm <sup>3</sup>
ETRR-2	Prismatic	6,5x6,5x80 cm.	3380.00
TRR-1/M1	Cylindrical	R = 5.5 cm, H = 60 cm	5701.98
IRT-T (running)	Cylindrical	R = 4 cm, H = 55 cm	2764.60
IRT-T (new considered)	Cylindrical	R = 6.9 cm, H = 50 cm	7474.77

As we can see, the productivity of the new installation significantly exceeds both the existing technology at the IRT-T reactor as well as at the other considered reactors. It should be noted that when implementing the technology of irradiation of semiprecious stones, experimental studies on the experimental channel directly with samples of semiprecious stones are required; this is due to many assumptions adopted in the calculation of both energy release and effective heat conductivity. It is also necessary to calculate the effect of the irradiated container on the change in reactivity during reactor operation. In addition, the next step in the study is the task of optimizing the installation, expressed in the calculated and experimental determination of the best quality conditions for the irradiation of materials, which would ensure the high economic value of the finished product.

## **6 Financial management, resource efficiency and resource saving**

The purpose of this section discusses the issues of competitiveness, resource efficiency and resource saving, as well as financial costs regarding the object of study of Master's thesis. Competitiveness analysis is carried out for this purpose. SWOT analysis helps to identify strengths, weaknesses, opportunities and threats associated with the project, and give an idea of working with them in each particular case. For the development of the project requires funds that go to the salaries of project participants and the necessary equipment, a complete list is given in the relevant section. The calculation of the resource efficiency indicator helps to make a final assessment of the technical decision on individual criteria and in general.

### **6.1 Competitiveness analysis of technical solutions**

In order to find sources of financing for the project, it is necessary, first, to determine the commercial value of the work. Analysis of competitive technical solutions in terms of resource efficiency and resource saving allows to evaluate the comparative effectiveness of scientific development. This analysis is advisable to carry out using an evaluation card.

First of all, it is necessary to analyze possible technical solutions and choose the best one based on the considered technical and economic criteria.

The position of the research under consideration and competitors is evaluated for each indicator on a five-point scale, where 1 is the weakest position and 5 is the strongest. The weights of indicators determined by you in the amount should be 1. Analysis of competitive technical solutions is determined by the formula:

$$C = \sum W_i \cdot P_i,$$

where:  $C$  – the competitiveness of research or a competitor;

$W_i$  – criterion weight;

$P_i$  – point of  $i$ -th criteria.

In this Master's thesis, a project is proposed on the alternative use of an experimental channel for irradiating semiprecious stones in it with a flux of fast neutrons. In addition, there are methods on the market for irradiating semiprecious

stones using a powerful source of gamma rays in a special installation or high-energy electrons in accelerators.

Thus, we will determine the competitiveness values, and based on the obtained values, in Table 1 we will present an evaluation card, which is an analysis of the competitiveness of the installation for irradiation of semiprecious stones and alternative methods for refinement of stones: gamma-ray irradiation (Competitor 1) and high-energy electron irradiation (Competitor 2). The different criteria for the model of expert evaluation are used. Evaluation map analysis presented in Table 1.

Table 1. Evaluation card for comparison of competitive technical solutions

Evaluation criteria <i>example</i>	Criterion weight	Points			Competitiveness Taking into account weight coefficients		
		$P_f$	$P_{i1}$	$P_{i2}$	$C_f$	$C_{i1}$	$C_{i2}$
1	2	3	4	5	6	7	8
<b>Technical criteria for evaluating resource efficiency</b>							
1. Energy efficiency	0.05	5	2	3	0.25	0.1	0.15
2. Reliability	0.1	5	5	5	0.5	0.5	0.5
3. Safety	0.25	3	3	4	0.75	0.75	1
4. Functional capacity	0.15	5	2	3	0.75	0.3	0.45
5. Ease of operation	0.03	3	4	4	0.09	0.12	0.12
6. Power requirement	0.1	3	5	4	0.3	0.5	0.4
<b>Economic criteria for performance evaluation</b>							
1. Development cost	0.05	5	4	3	0.25	0.2	0.15
2. Market penetration rate	0.05	5	2	2	0.25	0.1	0.1
3. Expected lifecycle	0.02	4	4	4	0.08	0.08	0.08
4. Induced radioactivity after irradiation	0.2	3	5	4	0.6	1	0.8
<b>Total</b>	<b>1</b>				3.82	3.65	3.75

Undoubtedly, the most important criterion is the radiation safety in the implementation of the technology. In this case, ensuring safety on electron accelerators is simpler than when implementing the technology under consideration with irradiation with reactor neutrons or a source of gamma rays. The induced activity of topazes after irradiation plays an equally important role: with a high value of induced activity, the exposure time before use by the consumer may be too high, which reduces the consumer value of the stones to zero.

From an economic point of view, when implementing the technology under consideration, the greatest productivity (functional capacity) of the plant for the refinement of stones is required. In this case, neutron irradiation occupies a leading role. Thus, it is clear that the technology in general exceeds the capabilities of competitors. This, in fact, determines the distribution of the technology in question on the market.

## **6.2 SWOT analysis**

Complex analysis solution with the greatest competitiveness is carried out with the method of the SWOT analysis: Strengths, Weaknesses, Opportunities and Threats. The analysis has several stages. The first stage consists of describing the strengths and weaknesses of the project, identifying opportunities and threats to the project that have emerged or may appear in its external environment. The second stage consists of identifying the compatibility of the strengths and weaknesses of the project with the external environmental conditions. This compatibility or incompatibility should help to identify what strategic changes are needed. SWOT analysis is presented in Table 2.

Table 2 – SWOT-analysis

	<p><b>Strengths:</b>  S1. Increase in the total production volume of semiprecious stones  S2. The increase in revenues.  S3. Using the potential of the reactor installation.  S4. Satisfying socially oriented needs.</p>	<p><b>Weaknesses:</b>  W1. Experimental confirmation of the results is required.  W2. Increase in expenses.  W3. Labor input.</p>
<p><b>Opportunities:</b>  O1. Entering new markets.  O2. High demand for semiprecious stones in the jewelry market  O3. Expanding the capabilities of the reactor installation.  O4. The growth of loyalty to the nuclear industry.</p>	<p>The results of the analysis of the interactive matrix of the project fields "Strengths and opportunities":  1. An increase in the operating time of semiprecious stones will allow reaching new customers.  2. The emergence of additional demand and financing, provided by the relevance of the topic.  3. The growth of capabilities of IRT-T.</p>	<p>The results of the analysis of the interactive matrix of the project fields "Weaknesses and opportunities":  1. Experimental confirmation required.  2. The costs of implementing the method can quickly pay off the income from the sale of the finished product.  3. The circle of consumers can be increased by entering new markets.</p>
<p><b>Threats:</b>  T1. End of operation of the IRT-T reactor installation.  T2. The likelihood of an increase in the operating time of semiprecious stones by competitors.  T3. Difficulty in implementing the method.  T4. A complete lack of demand in the future.</p>	<p>The results of the analysis of the interactive matrix of the project fields "Strengths and threats":  1. The increase in the potential of IRT-T, may possibly lead to an extension of the service life of reactor.  2. Current trends expressed in the depletion of natural topaz deposits allow us to conclude that the demand for the product will only grow in the future.</p>	<p>The results of the analysis of the interactive matrix of the project fields "Weaknesses and threats":  1. The complexity and high cost of the method are the main obstacles to its implementation  2. However, due to the depletion of the natural resources of semiprecious stones in the market, there is a strong increase in demand for semiprecious stones obtained by irradiation in the reactor. This allows the technology in question to be economically viable.</p>

Thus, having performed the SWOT analysis, we can conclude that at the moment the advantages of the developed model significantly prevail over its disadvantages. All existing imperfections can be easily eliminated using the above possibilities.

### 6.3 Project Initiation

The initiation process group consists of processes that are performed to define a new project or a new phase of an existing one. In the initiation processes, the initial

purpose and content are determined and the initial financial resources are fixed. The internal and external stakeholders of the project who will interact and influence the overall result of the research project are determined. Stakeholders of the project are presented in Table 3.

Table 3 – Stakeholders of the project

Stakeholder	Stakeholder's expectations
Division of nuclear fuel cycle, ESNT of TPU	A model on the basis of which it is possible to use the technology of treatment of semiprecious stones in the new vertical experimental channel of the IRT-T reactor

Table 4 provides necessary information of project goals and criteria for achieving these goals.

Table 4 – Purpose and results of the project

Purpose of project:	Creating the project on application of the large diameter vertical experimental channel of the IRT-T reactor for neutron irradiation of semiprecious stones
Expected results of the project:	Computer model, clearly describing physical processes during semiprecious stones treatment and possibility of applying such model in manufacture
Criteria for acceptance of the project result:	Compliance of calculated parameters with analytical prediction
Requirements for the project result:	Measurement error of simulation is less than 10%
	The model takes into account radioactive impurities in the atomic structure of topazes
	The radius of the irradiation container corresponds to the required temperature conditions
	The configuration of the thermal neutron filter corresponds to the necessary condition for the ratio of fast and thermal neutron fluxes

#### 6.4 The organizational structure of the project

It is necessary to solve the some questions: who will be part of the working group of this project, determine the role of each participant in this project, and prescribe the



functions of the participants and their number of labor hours in the project. This information is represented in Table 5

Table 5 – Organizational structure of the project

№	Participant	Role in the project	Functions	Labor time, hours.
1	Naymushyn A.G., associate professor of the division of nuclear fuel cycle, ESNT	Scientific advisor	Consulting	72
2	Brashchenko A.A., student	Engineer	Making the project on application of technology of semiprecious stones treatment in the IRT-T reactor	702
			Total	774

Project limitations are all factors that can be as a restriction on the degree of freedom of the project team members. Project limitations are presented in Table 6.

Table 6 – Project limitations

<b>Factors</b>	<b>Limitations / Assumptions</b>
3.1. Project's budget	249652.66 rub
3.1.1. Source of financing	National Research Tomsk Polytechnic University
3.2. Project timeline:	01.02.2020-22.05.2020
3.2.1. Date of approval of plan of project	05.02.2020
3.2.2. Completion date	22.05.2020

As part of planning a science project, you need to build a project timeline and a Gantt Chart. Project Schedule is presented in Table 7.

Table 7 – Project Schedule

№ работы	Job title	Duration, working days	Start date	Date of completion	Participants
1	Development of technical specifications	2	1.02.2020	3.02.2020	Scientific advisor
2	Drafting and approval of technical specifications	2	3.02.2020	5.02.2020	Scientific advisor
3	The choice of research direction	5	5.02.2020	10.02.2020	Scientific advisor, student
4	Selection and study of materials on the topic	2	10.02.2020	12.02.2020	Student
5	Work scheduling	1	12.02.2020	13.02.2020	Scientific advisor, student
6	Studying the capabilities of the calculation model	1	13.02.2020	14.02.2020	Student
7	Mastering calculation methods in practice	1	14.02.2020	14.02.2020	Student
8	Performing calculations	36	15.02.2020	30.03.2020	Student
9	Obtained data analysis	2	28.03.2020	30.03.2020	Student
10	Summary and assessment of results	1	30.03.2020	30.03.2020	Scientific advisor, student
11	Compilation of an explanatory note	60	14.02.2020	25.04.2020	Student
12	The verification of the results	1	26.04.2020	27.04.2020	Scientific advisor, student
13	Preparation to submitting	26	27.04.2020	22.05.2020	Student

Total 117 days for the student (excluding preparation for defense) and 12 days for the supervisor. Taking into account the daily working time of 6 hours, the number of working hours for a student is 702, for a supervisor 72.

A Gantt chart, or harmonogram, is a type of bar chart that illustrates a project schedule. This chart lists the tasks to be performed on the vertical axis, and time intervals on the horizontal axis. The width of the horizontal bars in the graph shows the duration of each activity.

Table 8 – Gantt chart

№	Activities	Participants	T <sub>c</sub> , days	Duration of the project													
				February			March			April			May				
				1	2	3	1	2	3	1	2	3	1	2	3		
1	Development of technical specifications	Scientific advisor	2	█													
2	Drafting and approval of technical specifications	Scientific advisor	2	█													
3	The choice of research direction	Scientific advisor, student	5	█	█												
4	Selection and study of materials on the topic	Student	2		█												
5	Work scheduling	Scientific advisor, student	1		█												
6	Studying the capabilities of the calculation model	Student	1		█												
7	Mastering calculation methods in practice	Student	1		█												
8	Performing calculations	Student	36			█	█	█	█	█	█	█	█	█	█	█	█
9	Obtained data analysis	Student	2														█
10	Summary and assessment of results	Scientific advisor, student	1														█
11	Compilation of an explanatory note	Student	60			█	█	█	█	█	█	█	█	█	█	█	█
12	The verification of the results	Scientific advisor, student	1														█
13	Preparation to submitting	Student	26														█

█ – Scientific advisor

█ – Student

## 6.5 Scientific and technical research budget

The amount of costs associated with the implementation of this work is the basis for the formation of the project budget. This budget will be presented as the lower limit of project costs when forming a contract with the customer.

To form the final cost value, all calculated costs for individual items related to the manager and the student are summed.

In the process of budgeting, the following grouping of costs by items is used:

- Material costs of scientific and technical research;
- costs of special equipment for scientific work (Depreciation of equipment used for design);
- basic salary;
- additional salary;
- labor tax;
- overhead.

### 6.5.1 Calculation of material costs

The main work for the Master's thesis was carried out behind the computer in the dorm room. In this research work used laptop as workstation. The time spent at the laptop was 702 hours. Workstation power: 65 W. Energy costs are calculated by the formula:

$$C = P_{el} \cdot P \cdot F_{eq} = 702 \cdot 5.8 \cdot 0.065 = 264.65 \text{ rub,}$$

where  $P_{el}$  – power rates (5.8 rubles per 1 kWh);

$P$  – power of equipment, kW;

$F_{eq}$  – equipment usage time, hours.

Thus, the cost of electricity amounted to 264.65 rubles.

The software used in this work (Monte-Carlo Universal and Comsol Multiphysics) has a license provided and paid by TPU; therefore, the costs of acquiring a license are not taken into account in this work. In addition, material costs include the need to provide Internet access for 4 months (monthly fee for one month is 350 rubles).

In addition, this work item counts the cost of purchase of equipment used in carrying out the work. Special equipment used for work is included in the form of

depreciation for the period of use. The calculation of depreciation is carried out according to the formula:

$$A = \frac{H_A \cdot C \cdot T_0}{365 \cdot 100\%} = \frac{33 \cdot 43000 \cdot 117}{365 \cdot 100\%} = 4548.58 \text{ rub,}$$

where  $A$  – depreciation charges, rub .;

$C$  – cost of equipment, rub;

$H_A = \frac{100}{T_{ex}} = 33\%$  – annual depreciation rate;

$T_{ex}$  – life expectancy, 3 years.

$T_{ex}$  – life expectancy, 3 years.

Table 10 - Depreciation

Name of equipment	Amount	C, rub	H <sub>A</sub> , %	T <sub>0</sub> , day	A, rub
Computer	1	43000	33	117	4548.58
Total, rub					4548.58

Table 11 – Material costs

Name	Unit	Amount	Price per unit, rub	Material costs. rub
1. Electrical energy	kW·h	702	5.8	264.65
2. Access to the Internet	rub/month	4	350	1400.00
Total, rub				1664.65

### 6.5.2 Basic salary

This point includes the basic salary of participants directly involved in the implementation of work on this research. The value of salary costs is determined based on the labor intensity of the work performed and the current salary system

The basic salary ( $S_b$ ) is calculated according to the following formula:

$$S_b = S_a \cdot T_w,$$

where  $S_b$  – basic salary per participant;

$T_w$  – the duration of the work performed by the scientific and technical worker, working days;

$S_a$  - the average daily salary of an participant, rub.

The average daily salary is calculated by the formula:

$$S_d = \frac{S_m \cdot M}{F_v},$$

where  $S_m$  – monthly salary of an participant, rub.;

$M$  – the number of months of work without leave during the year: at holiday in 48 days,  $M = 11.2$  months, 6 day per week;

$F_v$  – valid annual fund of working time of scientific and technical personnel (251 days).

Table 12 – The valid annual fund of working time

<b>Working time indicators</b>	
Calendar number of days	365
The number of non-working days	
- weekend	52
- holidays	14
Loss of working time	
- vacation	48
- sick absence	
The valid annual fund of working time	251

Monthly salary is calculated by formula:

$$S_{month} = S_{base} \cdot (k_{premium} + k_{bonus}) \cdot k_{reg},$$

where  $S_{base}$  – base salary, rubles;

$k_{premium}$  – premium rate;

$k_{bonus}$  – bonus rate;

$k_{reg}$  – regional rate.

Table 13 – Calculation of the base salaries

Performers	$S_{base}$ , rubles	$k_{premium}$	$k_{bonus}$	$k_{reg}$	$S_{month}$ , rub.	$S_d$ , rub.	$T_p$ , work days	$W_{base}$ , rub.
Associate professor	33600	1	1	1,3	43680	1949.07	12	23388.84
Engineer	17310				22503	1004.12	117	117482.04

### 6.5.3 Additional salary

This point includes the amount of payments stipulated by the legislation on labor, for example, payment of regular and additional holidays; payment of time associated with state and public duties; payment for work experience, etc.

Additional salaries are calculated on the basis of 10-15% of the base salary of workers:

$$W_{add} = k_{extra} \cdot W_{base},$$

where  $W_{add}$  – additional salary, rubles;

$k_{extra}$  – additional salary coefficient (10%);

$W_{base}$  – base salary, rubles.

The results of the calculation of the main and additional salaries of the performers of the research are presented in Table 14.

Table 14 - The salary of the performers of research work

The salary, rub	Project leader	Engineer
Basic	23388.84	117482.04
Additional	2338.88	11748.20
Total	25727.72	129230.24
Sum	154957.96	

### 6.5.4 Labor tax

Tax to extra-budgetary funds are compulsory according to the norms established by the legislation of the Russian Federation to the state social insurance (SIF), pension fund (PF) and medical insurance (FCMIF) from the costs of workers.

Payment to extra-budgetary funds is determined of the formula:

$$P_{social} = k_b \cdot (W_{base} + W_{add}) \quad (x)$$

where  $k_b$  – coefficient of deductions for labor tax.

In accordance with the Federal law of July 24, 2009 No. 212-FL, the amount of insurance contributions is set at 30%. Institutions conducting educational and scientific activities have rate - 27.1%.

Table 15 – Labor tax

	Project leader	Engineer
Coefficient of deductions	0.271	
Salary, rubles	25727.72	129230.24
Labor tax, rubles	6972.21	35021.95

### 6.5.5 Overhead costs

Overhead costs include other management and maintenance costs that can be allocated directly to the project. In addition, this includes expenses for the maintenance, operation and repair of equipment, production tools and equipment, buildings, structures, etc.

Overhead costs account 30% of the amount of base and additional salary of employees.

Overhead is calculated according to the formula:

$$C_{ov} = k_{ov} \cdot (W_{base} + W_{add}) \quad (x)$$

where  $k_{ov}$  – overhead rate.



Table 16 – Overhead costs

	Project leader	Engineer
Overhead rate	0.3	
Salary, rubles	25727.72	129230.24
Overhead, rubles	7718.32	38769.07

### 6.5.6 Formation of budget costs

The calculated cost of research is the basis for budgeting project costs. Determining the budget for the scientific research is given in the table .

Table 17 – Items expenses grouping

Name	Cost, rubles
1. Material costs	6213.23
2. Basic salary	140870.8
3. Additional salary	14087.08
4. Labor tax	41994.16
5. Overhead	46487.39
<b>Total planned cost</b>	<b>249652.66</b>

### 6.6 Evaluation of the comparative effectiveness of the project

Determination of efficiency is based on the calculation of the integral indicator of the effectiveness of scientific research. Its finding is associated with the definition of two weighted average values: financial efficiency and resource efficiency.

The integral indicator of the financial efficiency of a scientific study is obtained in the course of estimating the budget for the costs of three (or more) variants of the execution of a scientific study.

For this, the largest integral indicator of the implementation of the technical problem is taken as the calculation base (as the denominator), with which the financial values for all the options are correlated.

The integral financial measure of development is defined as:

$$I_{\phi}^p = \frac{\Phi_{pi}}{\Phi_{\max}},$$

where  $I_{\phi}^p$  – integral financial measure of development;

$\Phi_{pi}$  – the cost of the i-th version;

$\Phi_{\max}$  – the maximum cost of execution of a research project (including analogues).

The obtained value of the integral financial measure of development reflects the corresponding numerical increase in the budget of development costs in times (the value is greater than one), or the corresponding numerical reduction in the cost of development in times (the value is less than one, but greater than zero).

Since the development has one performance, then  $I_{\phi}^p = 1$ .

The integral indicator of the resource efficiency of the variants of the research object can be determined as follows:

$$I_m^a = \sum_{i=1}^n a_i b_i^a, I_m^p = \sum_{i=1}^n a_i b_i^p$$

where  $I_m$  – integral indicator of resource efficiency for the i-th version of the development;

$a_i$  – the weighting factor of the i-th version of the development;

$b_i^a, b_i^p$  – score rating of the i-th version of the development, is established by an expert on the selected rating scale;

$n$  – number of comparison parameters.

The calculation of the integral indicator of resource efficiency is presented in the form of table 17. The current project on the irradiation of topazes, as well as an analogue in the form of an installation for irradiating other semiprecious stones - amethysts, is considered.

Table 17 – Evaluation of the performance of the project

Criteria	Weight criterion	Points	
		Considered project	Analog
1. Installation cost	0,12	4	3
2. Safety	0,17	3	4
3. Material consumption	0,11	5	4
4. Radioactive impurities	0,08	4	2
5. Technology maturity	0,11	4	2
6. Ease in operation	0,08	3	3
7. Supply cost of raw material	0,13	5	4
<b>Economic criteria for performance evaluation</b>			
1. Price	0,1	4	3
2. Technology competitiveness	0,1	5	5
<b>Total</b>	1	37	30

The integral indicator of the development efficiency ( $I_{\text{финр}}^p$ ) is determined on the basis of the integral indicator of resource efficiency and the integral financial indicator using the formula:

$$I_{\text{финр}}^p = \frac{I_m^p}{I_\phi^p}, I_{\text{финр}}^a = \frac{I_m^a}{I_\phi^a} \text{ and etc.}$$

Comparison of the integral indicator of the current project efficiency and analogues will determine the comparative efficiency. Comparative effectiveness of the project:

$$\mathfrak{E}_{cp} = \frac{I_{\text{финр}}^p}{I_{\text{финр}}^a}.$$

Thus, the effectiveness of the development is presented in table 18.

Table 18 – Efficiency of development

№	Indicators	Points	
		Considered project	Considered project
1	Integral financial measure of development	1	1
2	Integral indicator of resource efficiency of development	4.09	3.42
3	Integral indicator of the development efficiency	4.09	3.42

Comparison of the values of integral performance indicators allows us to understand and choose a more effective solution to the technical problem from the standpoint of financial and resource efficiency.

## **7. Social responsibility**

### **7.1 Introduction**

The project is being developed to use the vertical experimental channel of the IRT-T nuclear research reactor for irradiating semiprecious stones by simulation on PC. Based on the requirements for irradiated samples (neutronic and temperature requirements), a container was developed that made it possible to irradiate samples in the experimental channel of a research nuclear reactor, and the induced activity of stones after irradiation was evaluated.

Simulation is performed using a personal computer and specialized software packages (MCU, COMSOL Multiphysics, MS Office) and does not require physical prototypes of the designed device. The user of the designed device is the IRT-T research nuclear reactor. For the most part, consumers of irradiated samples are manufacturers of precious jewelry.

In the section “Social Responsibility”, hazardous and harmful factors affecting the research process are examined, legal and organizational issues, as well as emergency measures are considered. Ecological safety is considered from the side of the influence of the designed research object on the environment.

### **7.2 Legal and organizational items in providing safety**

Nowadays one of the main ways to radical improvement of all prophylactic work referred to reduce Total Incidents Rate and occupational morbidity is the widespread implementation of an integrated Occupational Safety and Health management system. That means combining isolated activities into a single system of targeted actions at all levels and stages of the production process.

Occupational safety is a system of legislative, socio-economic, organizational, technological, hygienic and therapeutic and prophylactic measures and tools that ensure the safety, preservation of health and human performance in the work process [1]. According to the Labor Code of the Russian Federation, every employee has the right:

- to have a workplace that meets Occupational safety requirements;

- to have a compulsory social insurance against accidents at manufacturing and occupational diseases;
- to receive reliable information from the employer, relevant government bodies and public organizations on conditions and Occupational safety at the workplace, about the existing risk of damage to health, as well as measures to protect against harmful and (or) hazardous factors;
- to refuse carrying out work in case of danger to his life and health due to violation of Occupational safety requirements;
- be provided with personal and collective protective equipment in compliance with Occupational safety requirements at the expense of the employer;
- for training in safe work methods and techniques at the expense of the employer;
- for personal participation or participation through their representatives in consideration of issues related to ensuring safe working conditions in his workplace, and in the investigation of the accident with him at work or occupational disease;
- for extraordinary medical examination in accordance with medical recommendations with preservation of his place of work (position) and secondary earnings during the passage of the specified medical examination;
- for warranties and compensation established in accordance with this Code, collective agreement, agreement, local regulatory an act, an employment contract, if he is engaged in work with harmful and (or) hazardous working conditions.

The labor code of the Russian Federation states that normal working hours may not exceed 40 hours per week, the employer must keep track of the time worked by each employee.

Rules for labor protection and safety measures are introduced in order to prevent accidents, ensure safe working conditions for workers and are mandatory for workers, managers, engineers and technicians.

### **7.3 Basic ergonomic requirements for the correct location and arrangement of researcher's workplace**

The workplace when working with a PC should be at least 6 square meters.

The legroom should correspond to the following parameters: the legroom height is at least 600 mm, the seat distance to the lower edge of the working surface is at least 150 mm, and the seat height is 420 mm. It is worth noting that the height of the table should depend on the growth of the operator.

The following requirements are also provided for the organization of the workplace of the PC user. The design of the working chair should ensure the maintenance of a rational working posture while working on the PC and allow the posture to be changed in order to reduce the static tension of the neck and shoulder muscles and back to prevent the development of fatigue.

The type of working chair should be selected taking into account the growth of the user, the nature and duration of work with the PC. The working chair should be lifting and swivel, adjustable in height and angle of inclination of the seat and back, as well as the distance of the back from the front edge of the seat, while the adjustment of each parameter should be independent, easy to carry out and have a secure fit.

#### **7.4 Occupational safety**

A dangerous factor or industrial hazard is a factor whose impact under certain conditions leads to trauma or other sudden, severe deterioration of health of the worker [1]. A harmful factor or industrial health hazard is a factor, the effect of which on a worker under certain conditions leads to a disease or a decrease in working capacity.

##### **7.4.1 Analysis of harmful and dangerous factors that can create object of investigation**

The object of research is the design of an experimental channel with the aim of using it at the IRT-T research nuclear reactor for irradiating semiprecious stones by simulation on PC. Therefore object of investigation itself cannot cause harmful and dangerous factors.

We can consider harmful and dangerous factors that can occur when implementing this technology in practice. The casing of the experimental channel does not pose a threat to the environment, since the materials that are provided for its manufacture are not activated when they are irradiated with ionizing radiation.

A threat to the environment may be, firstly, an irradiation container made with a sputtering of boron carbide, which may have induced activity after irradiation, and secondly, irradiated semiprecious stones. For this purpose, the container and irradiated stones are kept in specialized rooms in accordance with the established radiation safety rules. So, in this work, it was calculated that the delay time for the stones before use by the consumer is 342 days.

#### **7.4.2. Analysis of harmful and dangerous factors that can arise at workplace during investigation**

The working conditions in the workplace are characterized by the presence of hazardous and harmful factors, which are classified by groups of elements: physical, chemical, biological, psychophysiological. The main elements of the production process that form dangerous and harmful factors are presented in Table 19.

Table 19 - Possible hazardous and harmful factors

Factors (GOST 12.0.003-2015)	Work stages			Legal documents
	Development	Manufacture	Exploitation	
1. Deviation of microclimate indicators	+	+	+	Sanitary rules 2.2.2 / 2.4.1340–03. Sanitary and epidemiological rules and regulations "Hygienic requirements for personal electronic computers and work organization."
2. Excessive noise		+	+	Sanitary rules 2.2.1 / 2.1.1.1278–03. Hygienic requirements for natural, artificial and combined lighting of residential and public buildings.
3. Increased level of electromagnetic radiation	+	+	+	Sanitary rules 2.2.4 / 2.1.8.562–96. Noise at workplaces, in premises of residential, public buildings and in the construction area.



Table 19 – Continuation

4. Insufficient illumination of the working area		+	+	Sanitary rules 2.2.4.548–96. Hygienic requirements for the microclimate of industrial premises.
5. Abnormally high voltage value in the circuit, the closure which may occur through the human body	+	+	+	

The following factors effect on person working on a computer:

– physical:

- temperature and humidity;
- noise;
- static electricity;
- electromagnetic field of low purity;
- illumination;
- presence of radiation;

– psychophysiological:

- psychophysiological dangerous and harmful factors are divided into:
  - physical overload (static, dynamic)
  - mental stress (mental overstrain, monotony of work, emotional overload).

### **Deviation of microclimate indicators**

The air of the working area (microclimate) is determined by the following parameters: temperature, relative humidity, air speed. The optimum and permissible values of the microclimate characteristics are established in accordance with [2] and are given in Table 20.

Table 20 - Optimal and permissible parameters of the microclimate

Period of the year	Temperature, °C	Relative humidity, %	Speed of air movement, m/s
Cold and changing of seasons	23-25	40-60	0.1
Warm	23-25	40	0.1

### **Excessive noise**

Noise and vibration worsen working conditions, have a harmful effect on the human body, namely, the organs of hearing and the whole body through the central nervous system. It results in weakened attention, deteriorated memory, decreased response, and increased number of errors in work. Noise can be generated by operating equipment, air conditioning units, daylight illuminating devices, as well as spread from the outside. When working on a PC, the noise level in the workplace should not exceed 50 dB.

### **Increased level of electromagnetic radiation**

The screen and system blocks produce electromagnetic radiation. Its main part comes from the system unit and the video cable. According to [2], the intensity of the electromagnetic field at a distance of 50 cm around the screen along the electrical component should be no more than:

- in the frequency range 5 Hz - 2 kHz - 25 V/m;
- in the frequency range 2 kHz - 400 kHz - 2.5 V/m.

The magnetic flux density should be no more than:

- in the frequency range 5 Hz - 2 kHz - 250 nT;
- in the frequency range 2 kHz - 400 kHz - 25 nT.

### **Abnormally high voltage value in the circuit**

Depending on the conditions in the room, the risk of electric shock to a person increases or decreases. Do not operate the electronic device in conditions of high humidity (relative air humidity exceeds 75% for a long time), high temperature (more than 35 °C), the presence of conductive dust, conductive floors and the possibility of

simultaneous contact with metal components connected to the ground and the metal casing of electrical equipment. The operator works with electrical devices: a computer (display, system unit, etc.) and peripheral devices. There is a risk of electric shock in the following cases:

- with direct contact with current-carrying parts during computer repair;
- when touched by non-live parts that are under voltage (in case of violation of insulation of current-carrying parts of the computer);
- when touched with the floor, walls that are under voltage;
- short-circuited in high-voltage units: power supply and display unit.

Upper limits for values of contact current and voltage is shown in Table 21.

Table 21 – Upper limits for values of contact current and voltage

	Voltage, V	Current, mA
Alternate, 50 Hz	2	0.3
Alternate, 400 Hz	3	0.4
Direct	8	1.0

### **Insufficient illumination of the working area**

Light sources can be both natural and artificial. The natural source of the light in the room is the sun, artificial light are lamps. With long work in low illumination conditions and in violation of other parameters of the illumination, visual perception decreases, myopia, eye disease develops, and headaches appear.

According to the standard, the illumination on the table surface in the area of the working document should be 300-500 lux. Lighting should not create glare on the surface of the monitor. Illumination of the monitor surface should not be more than 300 lux.

The brightness of the lamps of common light in the area with radiation angles from 50 to 90° should be no more than 200 cd/m, the protective angle of the lamps should be at least 40°. The safety factor for lamps of common light should be assumed to be 1.4. The ripple coefficient should not exceed 5%.

### **7.4.3 Justification of measures to reduce the levels of exposure to hazardous and harmful factors on the researcher**

#### **Deviation of microclimate indicators**

The measures for improving the air environment in the production room include: the correct organization of ventilation and air conditioning, heating of room. Ventilation can be realized naturally and mechanically. In the room, the following volumes of outside air must be delivered:

- at least 30 m<sup>3</sup> per hour per person for the volume of the room up to 20 m<sup>3</sup> per person;
- natural ventilation is allowed for the volume of the room more than 40 m<sup>3</sup> per person and if there is no emission of harmful substances.

The heating system must provide sufficient, constant and uniform heating of the air. Water heating should be used in rooms with increased requirements for clean air. The parameters of the microclimate in the laboratory regulated by the central heating system, have the following values: humidity 40%, air speed 0.1 m/s, summer temperature 20-25 °C, in winter 13-15 °C. Natural ventilation is provided in the laboratory. Air enters and leaves through the cracks, windows, doors. The main disadvantage of such ventilation is that the fresh air enters the room without preliminary cleaning and heating.

#### **Excessive noise**

In research audiences, there are various kinds of noises that are generated by both internal and external noise sources. The internal sources of noise are working equipment, personal computer, printer, ventilation system, as well as computer equipment of other engineers in the audience. If the maximum permissible conditions are exceeded, it is sufficient to use sound-absorbing materials in the room (sound-absorbing wall and ceiling cladding, window curtains). To reduce the noise penetrating outside the premises, install seals around the perimeter of the doors and windows.

#### **Increased level of electromagnetic radiation**

There are the following ways to protect against EMF:

- increase the distance from the source (the screen should be at least 50 cm from the user);
- the use of pre-screen filters, special screens and other personal protective equipment.

When working with a computer, the ionizing radiation source is a display. Under the influence of ionizing radiation in the body, there may be a violation of normal blood coagulability, an increase in the fragility of blood vessels, a decrease in immunity, etc. The dose of irradiation at a distance of 20 cm to the display is 50  $\mu\text{rem}$  / hr. According to the norms [2], the design of the computer should provide the power of the exposure dose of x-rays at any point at a distance of 0.05 m from the screen no more than 100  $\mu\text{R}$  / h.

Fatigue of the organs of vision can be associated with both insufficient illumination and excessive illumination, as well as with the wrong direction of light.

#### **Abnormally high voltage value in the circuit**

Measures to ensure the electrical safety of electrical installations:

- disconnection of voltage from live parts, on which or near to which work will be carried out, and taking measures to ensure the impossibility of applying voltage to the workplace;
- posting of posters indicating the place of work;
- electrical grounding of the housings of all installations through a neutral wire;
- coating of metal surfaces of tools with reliable insulation;
- inaccessibility of current-carrying parts of equipment (the conclusion in the case of electroporating elements, the conclusion in the body of current-carrying parts) [3].

#### **Insufficient illumination of the working area**

Desktops should be placed in such a way that the monitors are oriented sideways to the light openings, so that natural light falls mainly on the left. Also, as a means of protection to minimize the impact of the factor, local lighting should be installed due to insufficient lighting, window openings should be equipped with adjustable devices such as blinds, curtains, external visors, etc.

## **7.5 Ecological safety**

### **7.5.1 Analysis of the impact of the research object on the environment**

Most nuclear power plants release gaseous and liquid radiological effluents into the environment, which must be monitored. Civilians living within 80 km of a nuclear power plant typically receive about 0.1  $\mu\text{Sv}$  per year.

All reactors are required to have a containment building in according to international requirements. The walls of containment buildings are several feet thick and made of concrete and therefore can stop the release of any radiation emitted by the reactor into the environment

Large volumes of water are used during the process of nuclear power generation,. The uranium fuel inside reactors undergoes induced nuclear fission which releases great amounts of energy that is used to heat water. The water turns into steam and rotates a turbine, creating electricity. Nuclear plants are built near bodies of water.

All possible impact of nuclear power plant on environment is greatly reduced in operating regime by many safety precautions means. The most danger of nuclear energy come because of different sorts of disaster

### **7.5.2 Analysis of the environmental impact of the research process**

Process of investigation itself in the thesis do not have essential effect on environment. One of hazardous waste is fluorescent lamps. Mercury in fluorescent lamps is a hazardous substance and its improper disposal greatly poisons the environment.

Outdated devices goes to an enterprise that has the right to process wastes. It is possible to isolate precious metals with a purity in the range of 99.95–99.99 % from computer components. A closed production cycle consists of the following stages: primary sorting of equipment; the allocation of precious, ferrous and non-ferrous metals and other materials; melting; refining and processing of metals. Thus, there is an effective disposal of computer devices.

### **7.5.3 Justification of environmental protection measures**

Pollution reduction is possible due to the improvement of devices that produces electricity, the use of more economical and efficient technologies, the use of new

methods for generating electricity and the introduction of modern methods and methods for cleaning and neutralizing industrial waste. In addition, this problem should be solved by efficient and economical use of electricity by consumers themselves. This is the use of more economical devices, as well as efficient regimes of these devices. This also includes compliance with production discipline in the framework of the proper use of electricity.

Simple conclusion is that it is necessary to strive to reduce energy consumption, to develop and implement systems with low energy consumption. In modern computers, modes with reduced power consumption during long-term idle are widely used.

## **7.6 Safety in emergency**

### **7.6.1 Analysis of probable emergencies that may occur at the workplace during research**

The fire is the most probable emergency in our life. Possible causes of fire:

- malfunction of current-carrying parts of installations;
- work with open electrical equipment;
- short circuits in the power supply;
- non-compliance with fire safety regulations;
- presence of combustible components: documents, doors, tables, cable insulation, etc.

Activities on fire prevention are divided into: organizational, technical, operational and regime.

### **7.6.2 Substantiation of measures for the prevention of emergencies and the development of procedures in case of emergencies**

Organizational measures provide for correct operation of equipment, proper maintenance of buildings and territories, fire instruction for workers and employees, training of production personnel for fire safety rules, issuing instructions, posters, and the existence of an evacuation plan.

The technical measures include compliance with fire regulations, norms for the design of buildings, the installation of electrical wires and equipment, heating, ventilation, lighting, the correct placement of equipment.

The regime measures include the establishment of rules for the organization of work, and compliance with fire-fighting measures. To prevent fire from short circuits, overloads, etc., the following fire safety rules must be observed:

- elimination of the formation of a flammable environment (sealing equipment, control of the air, working and emergency ventilation);
- use in the construction and decoration of buildings of non-combustible or difficultly combustible materials;
- the correct operation of the equipment (proper inclusion of equipment in the electrical supply network, monitoring of heating equipment);
- correct maintenance of buildings and territories (exclusion of the source of ignition - prevention of spontaneous combustion of substances, restriction of fire works);
- training of production personnel in fire safety rules;
- the publication of instructions, posters, the existence of an evacuation plan;
- compliance with fire regulations, norms in the design of buildings, in the organization of electrical wires and equipment, heating, ventilation, lighting;
- the correct placement of equipment;
- well-time preventive inspection, repair and testing of equipment.

In the case of an emergency, it is necessary to:

- inform the management (duty officer);
- call the Emergency Service or the Ministry of Emergency Situations - tel. 112;
- take measures to eliminate the accident in accordance with the instructions.

## **7.7 Conclusions**

In this section about social responsibility the hazardous and harmful factors were revealed. All necessary safety measures and precaution to minimize probability of accidents and traumas during investigation are given.



Possible negative effect on environment were given in compact form describing main ecological problem of using nuclear energy.

It could be stated that with respect to all regulations and standards, investigation itself and object of investigation do not pose special risks to personnel, other equipment and environment.

### **7.8 References**

1. Federal Law "On the Fundamentals of Labor Protection in the Russian Federation" of 17.07.99 № 181 – FZ.

2. SanPiN 2.2.2 / 2.4.1340-03. Sanitary-epidemiological rules and standards "Hygienic requirements for PC and work organization".

3. GOST 12.1.038-82 Occupational safety standards system. Electrical safety.

4. Fire and explosion safety of industrial facilities. GOST R12.1.004-85 Occupational safety standards system. Fire safety

## Conclusion

In the course of this research work, the possibility of using the designed experimental channel in the IRT-T reactor as an installation for irradiating semiprecious stones using the example of topaz crystals was considered. As the calculation model, the experimental channel model, made in the MCU code, was used, which allows calculating various reactor parameters. The new model of the irradiation facility was based on the existing model of the irradiation container for irradiating silicon.

First, in this paper, an analysis of the numerical simulation methods of bulk systems is carried out, while the physical quantities characterizing bulk systems are considered. The main ones are the porosity and effective thermal conductivity of the system. The average sizes of stones under irradiation are considered, and the dependence of the porosity of the system on the average particle size in the bulk is considered. Various models for determining effective thermal conductivity are considered and the averaged temperature dependence of effective thermal conductivity is determined, which has the following form:  $\lambda_{eff} = 0.004559 \cdot t + 0.949387$ . Moreover, the average thermal conductivity along the radius of the container was determined by the theorem on the average value in the interval.

The next step of research considers thermal and resonant neutron filters. An aluminum container with a topaz crystal is coated with cadmium foil or boron carbide to isolate crystals from thermal neutrons. An analysis of various studies showed that the most effective irradiation occurs when the ratio of fast neutron to thermal flux should be  $k \geq 10$ . The data obtained for various thermal neutron filters indicate that it is more expedient to use an absorbing filter made of boron carbide, from which a cylindrical container is made, the radial and axial thickness of which is 3 mm. The ratio of fast to thermal neutron fluxes in this case is  $k = 125.286$ . The obtained value satisfies the necessary conditions for irradiation of topazes, which indicates the possibility of implementing this technology and the possibility of continuing further research on this topic.

After that, the temperature conditions in the designed container are determined, the energy release in the volume of irradiated stones is determined, and the maximum temperature in the irradiated container at different value radius of the container is calculated. It was determined that in order to comply with the necessary conditions for irradiation, so that the temperature in the container does not exceed 200 ° C, it is necessary to reduce the useful radius of the container from the original value 10.2 cm down to 7.2 cm.

The induced activity of the irradiated semiprecious stones is estimated. Various studies are analyzed, on the basis of which typical impurities in topazes are determined. The average value of the fast neutron fluence, which is necessary to give the crystals the desired shade, is equal to  $F = 10^{17}$  n/cm<sup>2</sup>. The corresponding irradiation time was determined, which for the flux density of fast neutrons with an energy of more than 1 MeV was 1.54 days. The delay time of irradiated stones before their use by consumers (until the induced activity decreased below 74 Bq/g) was determined, which amounted to  $t_d = 342$  days. It is found that this value substantially depends on the deposit of semiprecious stones, on the irradiation time, and on the neutron spectrum. So, with a significant proportion of resonant and thermal neutrons, the delay time can be of the order of several years, which nullifies the economic value of the technology.

Thus, we can conclude that the next step in the study should be the optimization of operating conditions during irradiation. So, experimental confirmation of the calculations, including energy release and temperature conditions, as well as a more accurate determination of the configuration of the filter system in order to reduce the fraction of resonant and thermal neutrons are necessary.

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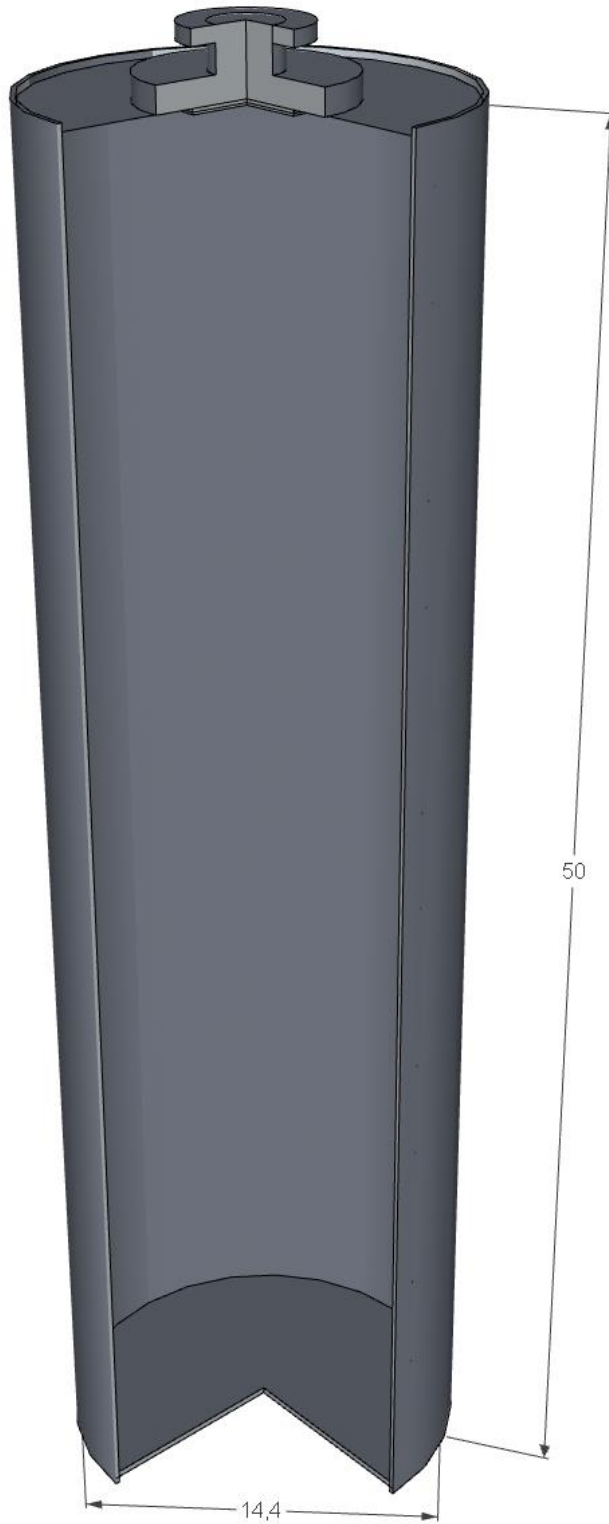
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## Appendix A

(required)

3D model of the irradiating container





## Appendix B

(required)

3D model of the experimental channel

