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Abstract. As part of the tasks to improve the nuclear safety of nuclear power plants, a new program code was developed. The CORIUMSITY program code developed, considered in this work, is intended to analyze the scenario in which an accident at a nuclear power plant is simulated with the melting of the core and the formation of the so-called “corium” - a mixture of nuclear and structural materials of the nuclear reactor core, formed as a result of thermal and mechanical impact during an accident. The CORIUMSITY program code, is intended to analyze several scenarios of different accidents, include an accident with reactor core melting. The functions of this code can help in solving many urgent nuclear safety problems. One of the main methods of operation of the CORIUMSITY code algorithms is the matrix exponential method, which consists in using a matrix function of a square matrix, in which as values are used indicators corresponding to nuclides from the CORIUMSITY code database. The program implements an iterative Euler method for solving the system of levels of nuclear fuel burnup. The CORIUMSITY code was verified with benchmark data to assess the accuracy of the calculation.

1. Introduction

At present, research and modeling of new generation reactors is being carried out all over the world, which significantly differ from commercial reactors currently in operation. Thus, the task of substantiating the safety of operation of new reactors is not only relevant, but also mandatory in the framework of the development of nuclear power in the world.

Because of the accidents that occurred at the end of the last century at nuclear power plants (the accident at the Three Mile Island nuclear power plant in 1979 and the accident at Chernobyl nuclear power plant in 1986) there was a demand for better analysis safety of reactor facilities. This analysis also includes the calculation and prediction of the consequences of accidents, including severe accidents with the melting of a reactor core, accidents of this type occurred at Three Mile Island and Chernobyl, and also at the Fukushima-Daiichi nuclear power plant in 2011.

Core melt accidents lead to the formation of corium - a solidified melt consisting of fuel, structural materials, remnants of regulators and etc. Modern reactor projects includes special structure – corium catcher [1], which, in case of accident, will be used to contain corium inside. Corium that located at the bottom of the reactor shaft is a powerful source of radiation and has a residual energy release. In

some situations, it may be necessary to extract corium from the remains of the reactor, for which it must be crushed and then extracted in small volumes, in this case the geometric characteristics of the corium and the uranium-water ratio change, which can potentially lead to criticality. Any manipulation of corium and its fragments is an extremely difficult task. Since corium is highly radioactive, it may affect environment radiological situation while locating in the damaged unit [2, 3] and during its transportation [4]. Determination of the composition and structure of the corium inside or outside the damaged core is a non-trivial task for any scientific organization. Such tasks are also complicated by the fact that it is necessary to take into account possible changes in the parameters of the corium when it is moved or any other effect on it. For the reasons described above, knowledge about the composition of corium and its neutron-physical characteristics is extremely important, and the accident at the Fukushima-1 NPP made this problem even more urgent. Determining the isotopic composition of the fuel at the time of the accident is the first step towards determining the isotopic composition of corium. The topic of calculating the burnup of nuclear fuel is well studied, the compositions of the fuel of industrial and designed reactors are known, as well as their plan of work - the history of burnup. For further calculation of the neutronic and radiation characteristics of the corium, it is necessary to determine with sufficient accuracy the concentrations of key fissile materials and fission products.

2. Using program codes to assess the structure and composition of the corium

Based on the information presented earlier, we can conclude that the safest and most relevant method for assessing the structure and neutron-physical characteristics of the corium is to calculate the isotopic composition using software.

2.1. Previously used software to evaluate the structure and neutron-physical parameters of corium

Functionaly-similar codes have been used to analyze samples from reactor core damaged during the Three Mile Island accident. Organisation for Economic Co-operation and Development (OECD) reports contatin usefull information and can be used as source of data, that important for this study. The process for assessing the structure of the corium was described in OECD reports «TMI-2 analysis exercise» [5] and «TMI-2 examination result» [6]. After taking corium samples and analyzing them, it was concluded that the special codes used to assess the structure of the corium used in the accident at the Three Mile Island NPP investigation did not give sufficiently accurate results. This is supported by the fact that the real structure of the corium, established by direct research during fuel extraction, did not coincide with the proposed structure estimated with the help of special codes. Hypothetical, estimated (by the special software) and confirmed TMI-2 reactor core end state are presented at figures 1-2.

A large number of works on determining the structure of the corium and the interaction of materials at high temperatures in the core are carried out using the old codes, some of which were developed after the accident at the Three Mile Island NPP. The functionality of these codes, the representatives of which can be called MAAP5 and MELCOR are insufficient to perform all tasks to ensure nuclear safety, in particular, the old codes are not capable of analyzing the isotopic composition of corium in the required volume.

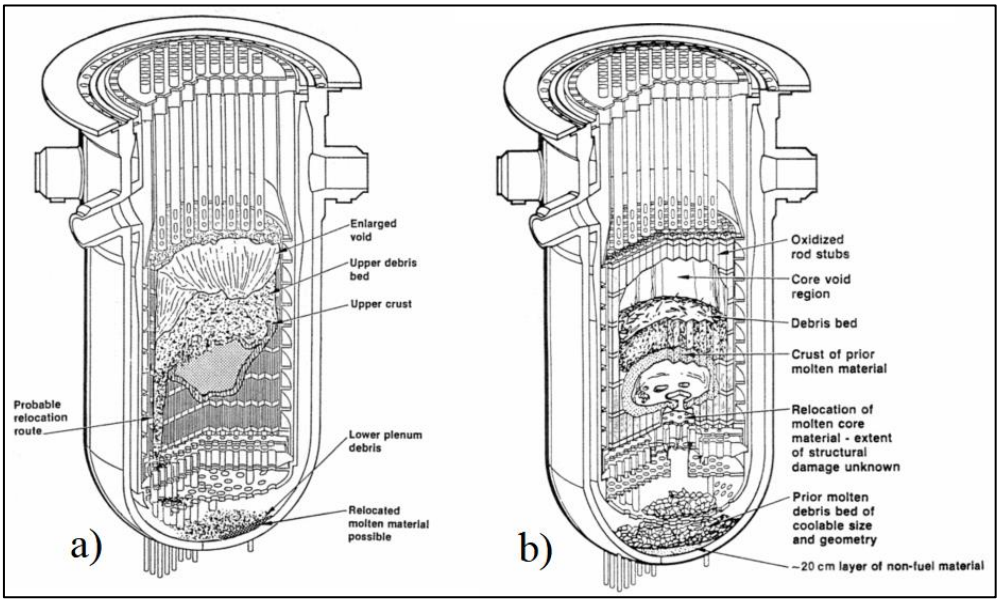

Figure 1. a) Hypothetical and b) estimated reactor end state after core boring 1986-1987.

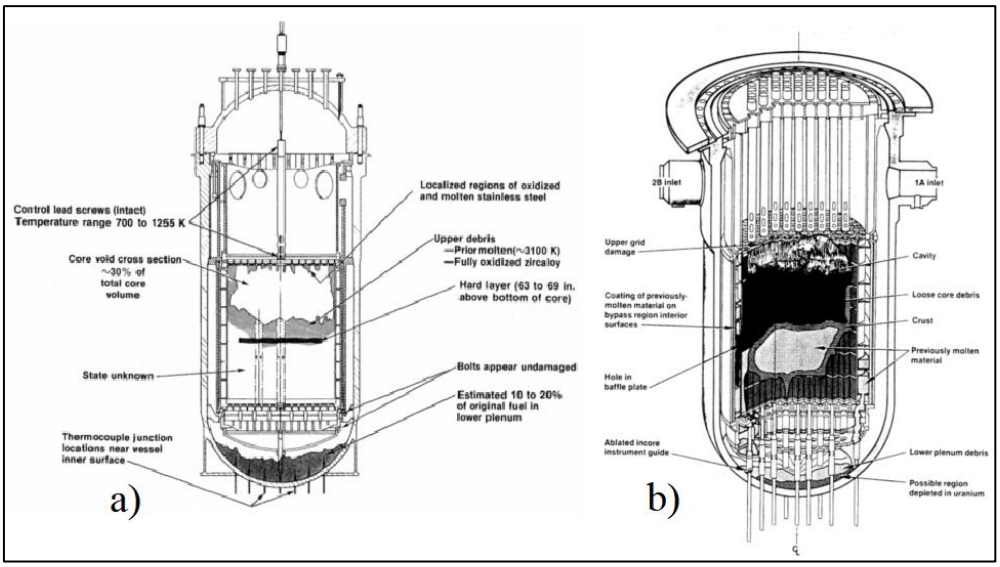

Figure 2. Known core state in the TMI-2 reactor vessel at the a) start (1985-1986) and at the end of defueling b) (1987-1990).

2.2. Modern software to evaluate the structure and neutron-physical parameters of corium

The problem of the accuracy of determining the structure of the corium formed as a result of an accident at a nuclear power plant is a topical topic with many modern studies in this area. Various scientific organizations around the world are working on this issue, with the aim of raising nuclear safety standards and developing technologies and recommendations for possible scenarios. Within the framework of these tasks, special codes are being developed. These works are carried out by various scientific organizations around the world and are exploring possible methods for analyzing the structure of the corium in various reactors and with using various methods.

Many modern software codes that can be used to solve the above problems implement CFD (Computational Fluid Dynamics) methods. In particular, one of the main representatives of such programs is the MIDAC code [7], which is being developed at the advanced nuclear power laboratory in Shanxi, China. However, this code is intended for the analysis of corium formation processes in

PWR reactors and uses CFD methods [8], which distinguishes it from the developed CORIUMSITY code, which uses methods of neutron-physical calculation of burnup for analysis.

Special codes are being developed to analyze specific tasks. For example, codes for analyzing the consequences of re-flooding of the reactor core after an accident [9], a code for analyzing specific chemical reconfigurations [10] and the code for complex numerical modeling of severe beyond design basis accidents with core melting [11].

2.3. Distinctive features of Coriumcity Code

The software tool for calculating the composition and structure of the corium formed as a result of an accident with the melting of the reactor core should have a wide functionality. In addition to the ability to analyze the isotopic composition of the corium and its fragments, the code should also have the ability to reconfigure nuclide-mixtures in the calculation process and should able to add or delete some elements during the formation of the corium. It is also important to have a functional for changing the geometry of the calculated models with the output of this information. The CORIUMSITY code was developed taking into account these requirements, which favorably distinguishes it from similar codes mentioned above. The CORIUMSITY program code, is intended to analyze several scenarios of different accidents, include an accident with reactor core melting. But one of the main assignment of this code is analysis of the corium - a mixture of nuclear and structural materials of the nuclear reactor core, formed as a result of thermal and mechanical impact during an accident.

The main area of application of the CORIUMSITY code is the assessment of the following parameters:

- radiation spectrum of corium formed as a result of an accident at a nuclear power plant;
- obtaining the distribution of the spectrum of alpha-beta-gamma and neutron radiation (neutron radiation greatly complicates the ability to study corium and take its samples);
- calculation of heat release in the corium at any time after the accident;
- accounting for the heterogeneous distribution of corium. Ability to obtain results on corium layers that form during melt flowdown;

Currently, CORIUMSITY code can be used in the tasks of assessing the structure and properties of the corium formed as a result of the accident at the Fukushima Daiichi NPP, as well as in the tasks of ensuring nuclear safety in the event of an accident at similar facilities (VVER and PWR reactors).

3. CORIUMSITY code development

Initially, the core code was developed to solve the problem of a subcritical system with corium particles and water. This task is an international benchmark designed to improve nuclear safety after the accident at the Fukushima nuclear power plant. In this benchmark, the criticality of a corium debris system was evaluated in order to prevent the organization of a critical mass of corium debris in reality. This problem has been studied all over the world in various scientific organizations [12]. In the course of work on this task [13-15], it was decided to develop a software tool that has wide functionality for solving nuclear safety problems.

During the development of the CORIUMSITY code, the functionality of the code is constantly expanding and currently includes other important functions. In particular, the possibility of dividing a mixture of nuclides into separate groups was added, for a more accurate analysis of various parameters, as well as the isolation of nuclides and fractions by type of radiation, which allows planning the processes of contact with corium or its fragments. One of the possible functionalities of the CORIUMSITY code is also the assessment of changes in the spectrum of corium, or individual fractions.

3.1. Algorithm of the CORIUMSITY code

One of the main methods of operation of the CORIUMSITY code algorithms is the matrix exponential method, which consists in using a matrix function of a square matrix, in which as values are used indicators corresponding to nuclides from the CORIUMSITY code database. The code uses as input data the concentration of nuclides and the parameters of the core (or other object) at the moment the corium starts to form. In the course of the code operation, it is necessary to calculate the composition and concentration of nuclides in the core in the pre-accident state, for which neutronic codes with the function of calculating burnup can be used (for example, the neutron-physical codes SERPENT and MCU).

Conventionally, the CORIUMSITY code calculation method is divided into three stages:

- preparing data for calculation;
- calculation;
- post-processing of results.

Let's take a closer look at each of these points. The algorithm of the CORIUMSITY code is shown in figure 3.

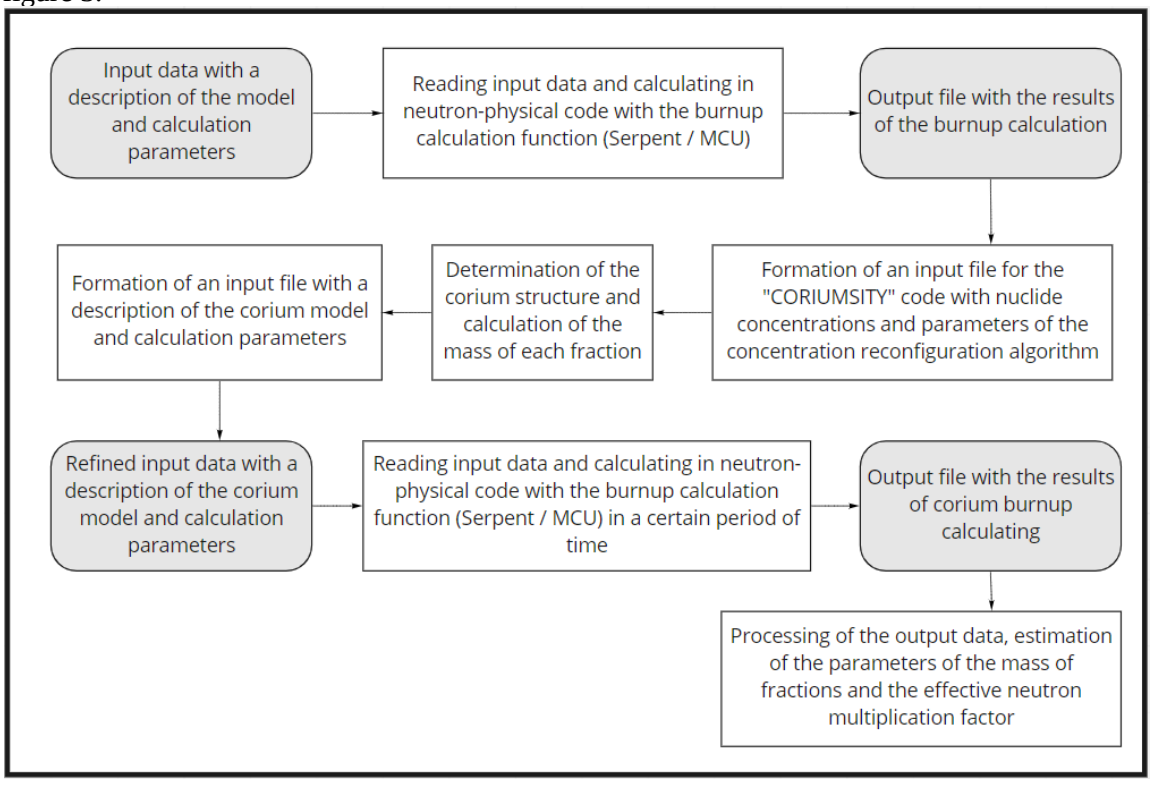

Figure 3. The algorithm of the CORIUMSITY code

3.1.1. *Preparing data for calculation.* At this stage, the calculation of the entire system (it can be a reactor or a test problem with a fuel assembly) is prepared for the calculation by the code, i.e. Neutron-physical analysis of the system is carried out, fuel burnup before immersion of a part of the concentrations in the CORIUMSITY code. In this case, a third-party module can be any neutron-physical code that supports the function of calculating fuel [16], or burnable absorber [17, 18] burnup. For example, Russian MCU (Kurchatov Institute) [19], Finnish Serpent (Finland, VTT) [20], or Japanese MVP [21] or American Scale (ORNL) [22] and others. All of these codes work independently of each other and of the CORIUMSITY app. However, after their development, a list of

isotopes is obtained with an indication of their non-zero concentrations (due to the fact that the fuel has already worked in the reactor for some time). This list of nuclides and their concentrations is placed into the CORIUMSITY program, and then the second stage begins.

To automatically transfer the received data, you can use plug-ins to interact with third-party software products. The CORIUMSITY program code allows you to do this due to the object-oriented approaches used in the design.

3.1.2. *Calculation.* The second stage implies direct calculation of the change in the isotopic composition during the accident and post-accident state. The concentration values obtained in the previous step are used as input data for the calculation. More details about exactly how, what methods are used to calculate the change in isotopic composition will be discussed below.

3.1.3. *Post-processing of results.* After the calculation, the results must be saved somewhere. CORIUMSITY saves the results to hard disk as output files in a text file in its own presentation. At figure 4 a part of the output file is presented, in which the resulting concentrations are stored at the time of calculation after the first step. This can be judged by the name of the file: "out.conc.stp1.dat". Here out is the keyword of the output file, dat is the extension of the output file (from the English word "data" - data), conc is the concentration, stp1 is the first step. For each step, only the number will change. The file "out.conc.stp1.layer1.dat" stores information about the concentrations for the layer with the conditional number 1. Thus, to find out the concentration after, say, the 50th step in the 8th layer of corium, we should open file "out. conc.stp50.layer8.dat ".

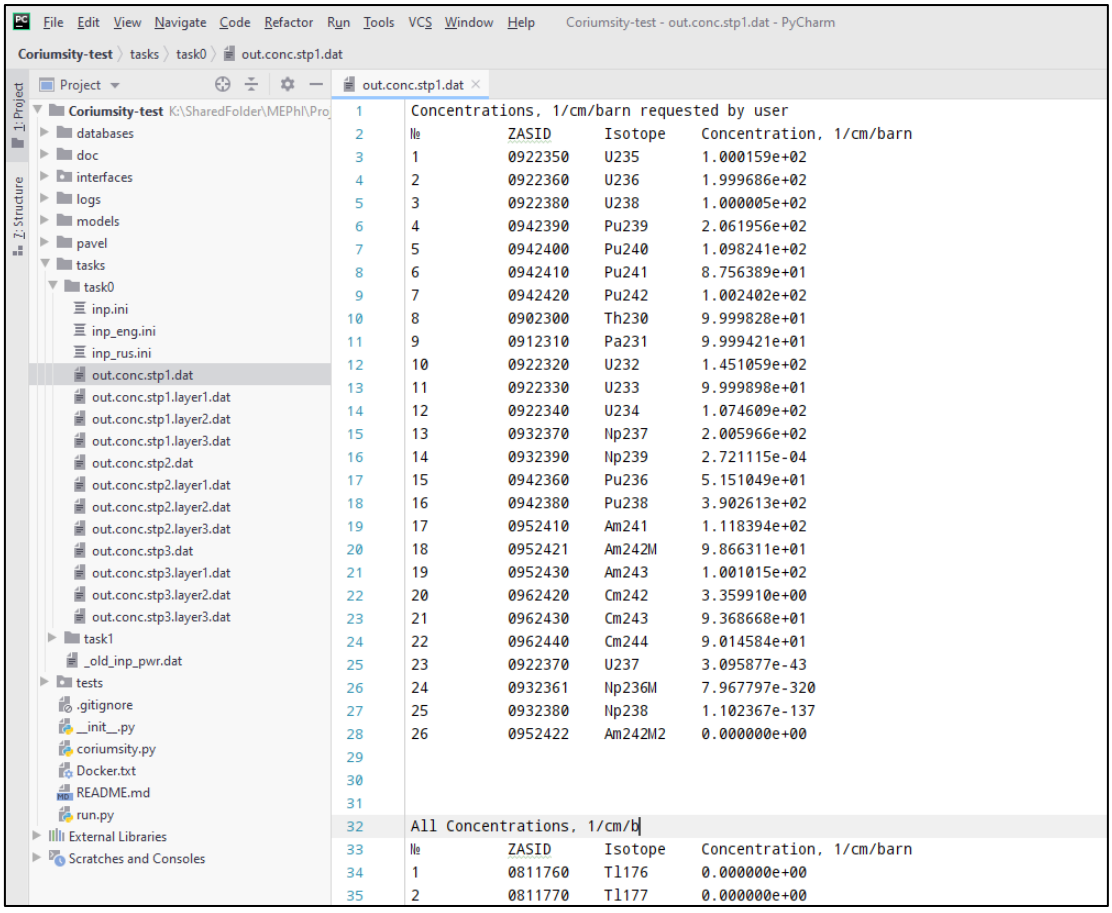

Figure 4. Part of the output file of the results of calculating the concentrations of the CORIUMSITY program

3.2. CORIUMSITY code method

The program implements an iterative Euler method for solving the system of levels of nuclear fuel burnup. The user must specify the size of the time step with which the problem is solved over the entire time interval, as well as the number of iterations of the division of the interval. In each such subinterval, all parameters, constants, and values of the burnup (decay) equation remain unchanged. After completion of the calculation on the subinterval, the values are recalculated taking into account the new received data. The size of the interval itself (the number of iterations), the time interval of the task must be selected by the user from physical considerations.

3.3. CORIUMSITY code verification

As a verification test for checking the correctness of the calculation by the matrix exponential method, was chosen the conditional problem of calculating the corium, for which the initial concentrations of all introduced nuclides are equal to 100 1/cm/b.

Such a simplification is necessary in order to understand after a given amount of time what percentage of the nuclide has decayed, and what nuclides have increased without the need to normalize to 100%, because the concentration is already 100. Time step: 1000 days. The number of corium layers is three. The number of time intervals of the Euler method was equal to 100. This problem was calculated using two methods: the matrix exponential method and the Euler method. The results were compared with the results of calculating the same problem using a similar code (reference solution). Table 1 shows the results of calculating this benchmark using the CORIUMSITY code using two calculation methods (matrix exponent and Euler's method), the results of calculating using the reference code, as well as the difference between the reference solution and the solution obtained using the CORIUMSITY code (matrix exponential method).

Table 1. A table with headings spanning two columns and containing notes.

Isotop	Coriumsity code Euler method	Coriumsity code matrix method	Referent code	Difference, %
U238	1.00E+02	1.00E+02	100	0.00
Pu242	1.00E+02	1.00E+02	100	0.00
U233	1.00E+02	1.00E+02	100	0.00
Am241	1.12E+02	1.12E+02	112	0.00
Th230	1.00E+02	1.00E+02	100	0.00
Pa231	1.00E+02	1.00E+02	100	0.01
Am243	1.00E+02	1.00E+02	100	0.01
U235	1.00E+02	1.00E+02	100	0.02
Pu241	8.77E+01	8.76E+01	87.6	0.04
Cm244	9.01E+01	9.01E+01	90	0.06
Pu240	1.10E+02	1.10E+02	110	0.07
Cm243	9.37E+01	9.37E+01	93.6	0.09
Am242M	9.87E+01	9.87E+01	98.8	0.14
Pu239	2.06E+02	2.06E+02	206	0.14
Np237	2.00E+02	2.00E+02	200	0.22
U236	1.61E+02	1.50E+02	152	1.30
U234	1.06E+02	1.02E+02	104	1.79

The table shows that the difference in the obtained concentrations after the accident for most isotopes does not exceed a percentage of the reference code for calculating isotope kinetics.

4. Conclusion

The CORIUMSITY code was developed, which has the full range of necessary functions to solve advanced nuclear safety problems. Taking into account the new standards after the accident at the Fukushima Daiichi NPP, the development of this code is an urgent task and this code can be used to solve many urgent problems. The code has been verified on an international benchmark and has shown good results. In the future, the code will be refined to expand the functionality of the program.

For full release of the CORIUMSITY code, it is necessary to carry out an additional verification of the results obtained using the CORIUMSITY code and experimental data from different benchmarks. For this, a dataset can be used to assess the structure of the corium formed as a result of a real accident at a nuclear power plant with a core melt. Similar accidents, have occurred at Three Mile Island and Fukushima Daiichi NPPs.

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