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Comparison of the results of conservative and realistic approaches to the analysis of radioactive release for LOCA of pressurized water VVER–440 and 1000 NPPs

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ABSTRACT

This paper presents the results of the assessment of the radiological consequences of LOCA at DBA and DEC-A for NPPs with VVER-440 and 1000 reactors using approaches that contribute to a realistic assessment of the radionuclide sources, taking into account the thermomechanical criterion of the gas gap activity release and the process of their transfer from the primary circuit to the environment. The results of the improved modelling are compared with conservative estimates.

1. Introduction

The reviews of safety analysis approaches after the Fukushima Daiichi Nuclear Power plant (FDNP) accident is motivated by the importance of strengthening the global assessment of the safety level of Nuclear Power Plants (NPPs) by considering specific situations more serious than those envisaged by the design of the NPPs. This has been stated by the IAEA (2016) through the definition of the Design Extension Conditions (DEC–A). The project "Reduction of Radiological Consequences of design basis and design extension Accidents" (R2CA) aims at assessments of radiological consequences (RC) of Design Basis Accidents (DBAs) and DEC-A reactor accidental situations, focusing on category of the Loss of Coolant Accidents (LOCAs).

The conservative simplified analysis of the safety of reactor unit in relation to the radiological consequences of emergency events of the LOCA type, which is presented in the article (Berezhnyi et al., 2023), involves the following approach in relation to two key points of the phenomenology of the transport of radionuclides:

- in a simplified manner the release of all the activity of isotopes in the primary circuit system due to the rupture to the containment space is considered, proportional to the leakage flow of the equivalent initial mass of the primary coolant;
- the thermomechanical criterion of damage to the fuel rods claddings is not taken into account, that is, in simplified manner the release of the activity of the gas gap content of all fuel rods is considered.

Some calculation results of a conservative assessment of radioactive release to the environment during LOCAs are given in the article (Berezhnyi et al., 2023). There is also a brief description of the reactor coolant system models for ATHLET (analysis of thermal-hydraulics of leaks and transients) code and containment models for the COCOSYS (containment code system) code, both for VVER–440 (water-water energetic reactor, Soviet design) and for VVER–1000 reactor units. The validation and verification data of the ATHLET code for the purposes of analysing transient processes associated with the deterioration of heat exchange in the core and the phenomenology of the primary circuit coolant leakage are given in (Lerchi et al., 2019, para.6.4; Hollands and Austregesilo, 2013). Validation and verification data of the COCOSYS code for the purposes of analysing the transport of isotopes and the phenomenology of processes in the containment system during transient processes, including those related to the coolant leakage from the primary circuit, are given in the (Arndt et al., 2020 para.2.5; Walter Klein-

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Heßling, 2019; Jan Husarcek and Ľubica Kubisova, 2019).

This paper is devoted to the results of a calculation studies regarding the possible reduction of conservatism in the assessment of radioactive release into the environment as a result of emergency processes associated with the primary circuit pipeline break within the containment (LOCA scenarios). The same calculation studies concern the assessment of the corresponding reduction of radiological impact on the population within the NPP sanitary protection zone.

Table 1 shows grouped data on the activity of radionuclides in the primary circuit, which are considered as part of the analysis of the safety of VVER-440 and VVER-1000 reactors for Ukrainian NPPs. These data are recommended by the fuel developer as being conservative in relation to the isotopic composition of the fuel for the assessment of the radiological consequences of accidents depending on the possible burnout of the fuel, its loading parameters, the type of fuel and the stage of the fuel cycle for the VVER-1000 and VVER-440 reactors. As can be seen from Table 1, the total activity of the gas gap is about 3 to 4 orders of magnitude greater than the activity of the coolant and the spike effect.

This paper examines the results of a computational study of improved modelling both in terms of the phenomenology of radionuclide transport in the primary circuit system, and in terms of the physical basis of evaluating the release of the activity of the fuel rods gas gap.

2. Modelling improvements and assumptions

Below are the main approaches and assumptions that were developed and adopted for computational modelling of a more realistic behaviour of isotopes on the way from the primary circuit to the containment through the cold leg break (at the reactor inlet nozzle). The modelling improvements listed below are made to the reactor plant models for ATHLET code and the containment models for COCOSYS code, a brief description of which is provided in article (Berezhnyi et al., 2023). These models were developed to analyse the safety of Ukrainian NPPs with VVER-1000 and VVER-440 reactors and were used at the stage of conservative assessment of the radiological consequences of the LOCA scenarios (article (Berezhnyi et al., 2023).

2.1. Modelling improvements

Modelling improvements relate to a more realistic assessment of activity release into the containment and further to the environment with a corresponding significant reduction in conservatism due to consideration of a set of physical processes on the path of radionuclide transport from the primary circuit to the containment and with consideration of the realistic conditions regarding the fraction of the gas gap activity release. Such modelling improvements are based on the following aspects:

- the BORTRANS module (Austregesilo et al., 2019 para.2.9) of the ATHLET reactor coolant system model is used for the equivalent modelling of radionuclide particles behaviour (physical and chemical processes and mechanisms) in the coolant of the primary circuit, namely:
- transport of radionuclides from the core by the primary coolant to the containment through the break,
- dilution of the radioactive primary coolant due to the injection from the Emergency Core Cooling Systems (ECCS),
- deposition of radionuclides in the volumes of the primary circuit due to the mechanism of the solubility of isotopes in the water coolant;
- generally accepted thermomechanical criteria (Courtright, 1979; Billone et al., 2009; Shewfelt, 1988) are applied to assess partial fuel damage with subsequent release of the corresponding part of the gas gap activity:
- an specific temperature criterion (800 °C) for damage to the fuel rods claddings is considered, the excess of which is accompanied by the release of gas gap activity,
- a detailed fuel assemblies model of the core is considered, which takes into account the non-uniformity of energy release across the fuel assemblies – for a more realistic estimate of the number of fuel assemblies for which the temperature condition for claddings damage is reached,
- the radial core energy distribution across the fuel assemblies is taken into account for a more realistic estimate of the fuel rods number of individual assemblies for which the criterion of the claddings damage temperature is reached;
- for the COCOSYS containment model a more detailed particle size classes spectrum is considered – a slight decrease in the release of activity in the environment due to more detailed and realistic modelling of the isotopes transport within the containment.

2.2. Modelling assumptions and principles

Modelling improvements to estimate FPs (fission products) release from primary circuit into containment for LOCA scenarios using the BORTRANS module (BORON mathematical model) of the ATHLET3.2/AC^2 code are based on the assumptions given below (Austregesilo et al., 2019 para.2.9; Lerchi et al., 2019 para.3.13):

1) The mathematical and physical interpretation of the BORTRANS module provides the possibility of thorough modelling of the phenomenology of the release and transport of radionuclides in the mass of the water coolant due to certain features of the module, namely:

- the inertia of the solute, as well as the energy transported by it, can be neglected for the mass and energy balances;
- the coolant properties are not altered due to presence of the solute – the presence of particles does not affect the thermohydraulic aspects of the simulation;
- the FILL (one of the types of hydrodynamic elements of the ATHLET code) junctions model is based on the assumption of a homogeneous flow and is also not governed by the transport equation; the FILL objects thus provide the possibility of modelling the release of particles to a user-specified volume at a specified time and in a specified

Table1
Radionuclides composition in primary coolant and fuel rods gas gap of VVER-440&1000 reactor core.

Isotopes group	Radionuclides	VVER-1000 Primary coolant and spike activity (Bq)	Fuel gas gap activity (Bq)	VVER-440 Primary coolant and spike activity (Bq)	Fuel gas gap activity (Bq)
Krypton	Kr–85,85 m,87,88	5.70E + 13	3.70E + 15	8.00E + 12	9.00E + 14
Xenon	Xe–133,135,135 *m*	3.40E + 13	3.16E + 16	8.80E + 12	1.05E + 16
Strontium	Sr–90	9.00E + 06	3.00E + 15	5.00E + 06	2.00E + 15
Rubidium	Ru–103,106	2.09E + 07	2.20E + 16	6.30E + 06	1.10E + 16
Iodine	I–131,132,133,134,135	1.50E + 14	3.70E + 16	2.90E + 13	1.35E + 16
Caesium	Cs–134,137	4.00E + 11	8.00E + 15	1.90E + 11	6.00E + 15
Cerium	Ce–141,144	1.07E + 08	8.00E + 16	4.30E + 07	4.00E + 16
Lanthanum	La–140	1.00E + 09	4.00E + 16	4.00E + 08	2.00E + 16
Total	–	2.41E + 14	2.25E + 17	4.60E + 13	1.04E + 17

amount; at the same time, deposition of particles in case of excess of their concentration of their solubility is possible only after their injection from a FILL junction, taking into account mixing with the main objects of the primary circuit topology, which avoids excessive non-physical deposition of isotopes, for example after the injection of spike effect or the gas gap activity (Austregesilo et al., 2019 para.4.2; para.5.1, para.5.11.1; Lerchi et al., 2019 para.10.1).

2) To simulate the entire spectrum of isotopes, one equivalent «user-defined» substance with the averaged properties of all radionuclides is introduced:

- for this substance, the averaged FP initial concentration in the primary coolant and the concentration of the spike and gas gap "artificial" injection, which result from the total activity of the isotopes, are determined and set;
- the activity-averaged maximum solubility is also determined and set for this substance, which affects the nature of particle deposition in the volumes of the primary circuit;
- this substance has neutron-physical properties of boric acid, but for the researched scenarios with core fuel loading at the beginning of fuel cycle and a significant loss of the coolant, the concentration of boron particles practically does not affect the thermohydraulic aspects of transient processes.

3) The initial activity of the primary coolant is set for volumes of the primary circuit model at steady-state, when mixing with the coolant in the reactor core is ensured; for systems disconnected at the steady state (e.g. ECCS), the equivalent solute concentration is set to zero.

4) The injection of the activity of the spike effect and of the gas gap (part of this activity is considered for some scenarios) is simulated at the beginning of the transient using the user-defined injection from the FILL element into core centre:

- the injection of a coolant with a concentration of particles that corresponds to the total activity of the spike effect or gas gap is simulated by an insignificant mass (0.01 kg and 1.0 kg respectively) over a short period of time (1.0 s), which, on the one hand, practically does not affect the phenomenology of the investigated emergency processes, and on the other hand, correlates with the rapid process of releasing the activity
- injection from the FILL component with a high concentration of particles does not lead to their excessive deposition due to the peculiarities of the ATHLET code and mathematical models for the FILL objects (Austregesilo et al., 2019 para.4.2; para.5.1, para.5.11.1; Lerchi et al., 2019 para.10.1);
- injection into the core centre simulates the average release of activity over the entire height of fuel rods and thus corresponds to the phenomenology of the subsequent transition of the isotope particles to the leakage place from the primary circuit to the containment.

5) For scenarios of the primary circuit leak, the assessment of the activity of the release into the containment is possible based on the mass balance of equivalent boron particles that are carried out of the topological system of the primary circuit.

6) For the containment model for the COCOSYS code (Arndt et al., 2020) the following modelling improvements are made in relation to reducing the conservatism of the LOCA radiological consequences evaluation:

- the updated distribution of isotopes releases in time after the modification of the model for the ATHLET code and after taking into account the thermomechanical criterion of damage to the fuel rods claddings is used as boundary conditions;
- the calculation time has been extended to 24 h for VVER–440 reactor plant and to 72 h for VVER–1000 reactor plant (guaranteed time to ensure the safety and autonomy of the specified NPP type) to take into account the entire spectrum of processes of nuclide transport from the containment to environment; in this way, the functions of the leakage flow from the primary circuit to the containment, as well as the flow characteristics of the ECCS, also have been extended;
- a more detailed particle size classes spectrum is considered, which provides a more detailed and realistic modelling of the isotopes transport inside the containment (Hollands and Austregesilo, 2013, para.8.6.1).

2.2.1. Equivalent modelling of radionuclides in primary circuit

The parameters of the equivalent model of the isotopes behaviour in the primary circuit for the ATHLET 3.2 code are considered below. As mentioned above, the entire spectrum of isotopes is modelled equivalently as one substance dissolved in the coolant using the BORTRANS module. Simulation of particles of equivalent isotopes in the primary circuit involves three constituent parts:

- isotopes in coolant of the primary circuit at nominal operation conditions – steady-state calculations;
- isotopes of spike effect activity – transient calculations;
- isotopes of fuel gas gap activity – transient calculations.

Model parameters of isotopes dissolved in the coolant at nominal operation conditions – solvent concentration in primary coolant:

$$C_{INIT} = SUM\left[\left(10^6 \times N_{NUCLD1.i}\right)/\left(SUM(N_{NUCLD1.i}) + N_{H2O}\right)\right](ppm),$$

where $N_{NUCLD1.i} = A_{INIT.i}/\lambda_i$ – particles number of i^{th} isotope; $A_{INIT.i}$ – initial i^{th} isotope activity in primary coolant (Bq); $\lambda_i = \ln(2)/T_{i.1/2}$ – decay constant of i^{th} isotope (s^{-1}); $T_{i.1/2}$ – half lifetime of i^{th} isotope (s), based on the extended map of all isotopes (Soti et al., 2018);

$N_{H2O}=(M_{H2O} \times N_A)/\mu_{H2O}$ – particles number of the primary coolant; M_{H2O} – primary circuit coolant mass at nominal operating conditions, with the exception of non-working systems of the primary circuit at the nominal state; initial value at 0.0 s for steady-state (kg); $\mu_{H2O} = 0.018$ kg/mole – water coolant molar mass; $N_A = 6.02214E + 23$ mol^{-1} – Avogadro Number.

Model parameters of isotopes released owing to spike effect at beginning of the transient – solvent concentration in spike effect artificial injection:

$$C_{SPIKE} = SUM\left[\left(10^6 \times N_{NUCLD2.i}\right)/\left(SUM(N_{NUCLD2.i}) + N_{FILL2}\right)\right](ppm),$$

where $N_{NUCLD2.i} = A_{SPIKE.i}/\lambda_i$ – particles number of i^{th} isotope; $A_{SPIKE.i}$ – spike effect activity of i^{th} isotope (Bq); must be noted, Table 1 shows sum of initial and spike effect activity; $N_{FILL2}=(M_{FILL2} \times N_A)/\mu_{H2O}$ – particles number of filled (injected) coolant for spike effect simulation; $M_{FILL2} =$ 0.01 kg – assumed injection mass for spike effect simulation; the adopted small value regarding to M_{H2O} practically does not affect the results of calculations.

Model parameters of isotopes released owing to fuel rod gas gap depressurization at the beginning of the transient – solvent concentration in gas gap artificial injection:

$$C_{GAP} = SUM\left[\left(10^6 \times N_{NUCLD3.i}\right)/\left(SUM(N_{NUCLD3.i}) + N_{FILL3}\right)\right](ppm),$$

where $N_{NUCLD3.i} = F_{clad} \times A_{GAP.i}/\lambda_i$ – particles number of i^{th} isotope; $A_{GAP.i}$ – fuel gas gap activity of i^{th} isotope (Bq); F_{clad} – fraction of damaged fuel rod claddings according to thermomechanical criterion (the definition of this parameter is considered in para.1.2.2 of this article); $N_{FILL3}=(M_{FILL3} \times N_A)/\mu_{H2O}$ – particles number of filled (injected) coolant for gas gap activity simulation; $M_{FILL3} = 1.0/0.5$ kg – assumed injection mass for gas gap release simulation (for VVER-1000/440 respectively); the adopted small value regarding to M_{H2O} practically does not affect the results of calculations.

For all calculation analysed at steady-state and transient stages, the model parameter such as the maximum solubility (averaged by activity) of all isotopes group for one modelled solute in the coolant is used. When the concentration of particles in any volume of the model exceeds the value of the maximum solubility, their deposition occurs:

$$S_{AVE.MAX} = SUM(A_{.i} \times S_{MAX.i})/SUM(A_{.i})(ppm),$$

where $A_{.i} = A_{INIT.i} + A_{SPIKE.i} + F_{clad} \times A_{GAP.i}$ – total activity of ith isotope (Bq); F_{clad} – fraction of damaged fuel rod claddings according to thermomechanical criterion (the definition of this parameter is considered in para.1.2.2 of this article); $S_{MAX.i}=(10^6 \times N_{ISO.i})/(SUM(N_{ISO.i}) + N_{WAT.})$ – maximum solubility of ith isotope (ppm); $N_{ISO.i}=(10^{-6} \times SLB_{MAX.i} \times N_A)/\mu_i$ – number of particles of ith isotope into 1 kg of water; $SLB_{MAX.i}$ – maximum solubility of ith isotope based on data (Card and Jansen, 1975) on the «ideal» chemical solubility of substances in pure water (mg/l); these values are somewhat conservative overestimated, but cover uncertainty in other aspects of modelling; $N_{WAT.} = N_A/\mu_{H2O} = 3.346E + 25$ – number of particles of 1 kg of water.

2.2.2. Evaluation of fraction of the fuel gas gap activity release

One of the main aspects of the improved modelling, which provides for more realistic conditions for transport of radionuclides from the primary circuit to the containment through the break, is the consideration of the thermomechanical criterion of damage of the fuel claddings for a more realistic assessment of the fraction of the gas gap activity release.

With regard to the proven practice of assessing the damage of fuel claddings during the LOCAs, the minimum temperature of the outer surface of claddings at which the formation of micro cracks occurs, i.e. the beginning of damage, is equal to 800 °C (Shewfelt, 1988). When the temperature reaches about 800 °C, zirconium in claddings starts to transform from alpha to the beta phase (Billone et al., 2009). At the same time, the oxidation reaction starts to accelerate and the growth of the oxide scale becomes significant. That is, a temperature of 800 °C is the lower limit of the start of an active steam-zirconium reaction with subsequent damage to the fuel claddings (Courtright, 1979).

The selected criterion 800 °C depends on the conditions of modelling the phenomenology of processes with the deterioration of the conditions of heat removal from the core during the LOCA scenarios using the model for the ATHLET code. Mathematical models for the ATHLET code, which simulate various physical processes in the reactor system, have some uncertainty and a degree of deviation from the dynamics of the processes in the real system. Fig. 1 shows a comparison of the calculated value of the claddings temperature, taking into account the results of the uncertainty analysis of the input data and mathematical models for the ATHLET 3.2 code and the experimental value for the process associated with the primary circuit leakage. As can be seen from Fig. 1, the calculated forecasting of the claddings temperature using the ATHLET 3.2 code assumes a greater value of both the peaks of the temperature and their duration. Regarding the maximum peak temperature, the ATHLET code predicts about 13 % higher value compared to experimental measurements (Lerchi et al., 2019 para.6.4). Thus, the use of models for the ATHLET code within the simulation of LOCA scenarios has a certain degree of conservatism due to the overestimation of the claddings temperature, therefore the selected criterion of 800 °C is provided with a conservative margin regarding the uncertainty of the assessment of the conditions for reaching this temperature. The same conclusions can be form regarding earlier versions of the ATHLET code. For example, for the ATHLET 2.2 code, there is also an overestimation of the value of the claddings temperature in comparison with experimental measurements for the primary circuit coolant leakage scenarios (Hollands and Austregesilo, 2013).

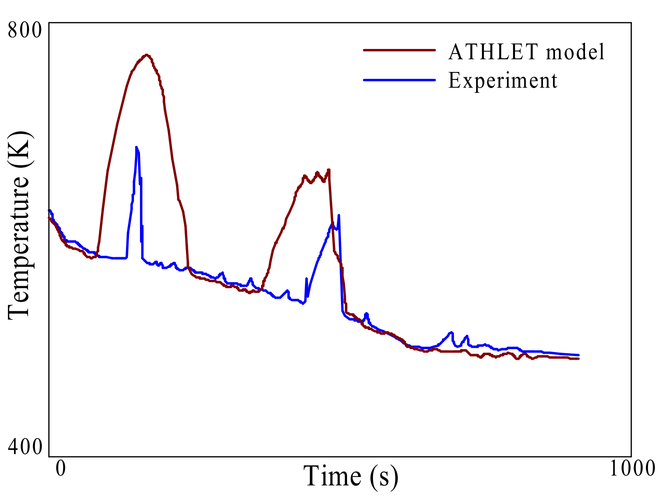

Fig. 1. Comparison of the experimental and calculated value of the claddings temperature for the LOCA scenario within the validation of the ATHLET 3.2 code (Lerchi et al., 2019, Fig. 6–1).

Thus, in the calculated scenarios for which the maximum value of the temperature of the fuel rods claddings of about 800 °C is not reached, the claddings are not damaged. That is, for scenarios with such conditions, the release of gas gap activity is not considered. According to the results of previous calculation analyses, part of which is given in paper (Berezhnyi et al., 2023), the accident scenarios in which the conditions for damage to the fuel rods claddings are achieved are as follows:

Item	VVER–1000 DBA	DEC–A	VVER–440 DBA	DEC–A
1	CL guillotine break with a diameter of 2 × 850 mm	CL guillotine break with a diameter of 2 × 850 mm	CL guillotine break with a diameter of 2 × 500 mm	–
2	CL break with a diameter of 350 mm	–	–	–

Note: CL – cold leg

For this scenarios in which the maximum temperature of the fuel claddings is reached to the value of their damage criterion (about 800 °C), additional detailed calculations were performed to determine the fraction of damaged rods. The improvement of modelling regarding the estimation of the fraction of damaged rods are based on the following approaches:

- In order to determine the number of fuel assemblies for which the maximum temperature of the fuel rods claddings above the 800 °C criterion is reached, in the Heat Conduction Objects (HCOs) model of the reactor core for the ATHLET code, the uneven distribution of energy release across all assemblies is taken into account (K_q coefficient). This provides a detailed fuel model of the core with corresponding detailed data on the claddings temperature. The HCOs model of fuel assemblies is grouped according to the value of K_q.
- At the stage of preliminary calculations of LOCAs, the power distribution parameters of a number of actual fuel loadings of Ukrainian NPPs were analysed. Fuel loadings were selected for which the criterion of 800 °C was reached for the largest part of assemblies. It was found that the criterion was met for assemblies with K_q exceeding approximately 1.2 and 1.3 for the VVER-1000 and VVER–440 reactors, respectively. Such fuel loadings are typical for the beginning of the fuel cycle. It should be noted that fuel loadings with the maximum allowable values of K_q (given in the reports on the justification of loadings) show in LOCAs a smaller amount of fuel assemblies with a temperature ≥ 800 °C compared to the actual loadings that are operated.
- For this work, the 28th fuel loading of the Khmelnitsky NPP Unit 1 (for VVER–1000) and the 35th fuel loading of the Rivne NPP Unit 2 (for VVER–440) are considered.

- Non-uniformity of energy release by assemblies also takes into account the maximum non-uniformity of energy release for the hot fuel assembly $K_{q.HA}$ and hot rod Kq.HR model (VVER design data for the fuel loads):
- o $K_{q.HA} = 1.05 \times 1.35 = 1.4175$ and $K_{q.HA} = 1.35$ – VVER–1000 reactor core at DBA and DEC–A calculations respectively; 1.35 – maximum permissible value of K_q value and 1.05 – engineering coefficient of inaccuracy of reactor heat power maintenance;
- o $K_{q.HA} = 1.02 \times 1.46 = 1.4892$ and $K_{q.HA} = 1.46$ – VVER–440 reactor core at DBA and DEC–A calculations respectively; 1.46 – maximum permissible value of K_q value and 1.02 – engineering coefficient of inaccuracy of reactor heat power maintenance;
- o Kq.HR = $1.16 \times 1.5 = 1.74$ and Kq.HR = 1.5 – VVER–1000 reactor core at DBA and DEC–A calculations respectively; 1.5 – maximum permissible coefficient of non-uniformity of energy release at core fuel rods and 1.16 – maximum value of engineering coefficient of reserve for local heat flux;
- o Kq.HR = $1.064 \times 1.62 = 1.72368$ and Kq.HR = 1.62 – VVER–440 reactor core at DBA and DEC–A calculations respectively; 1.62 – maximum permissible coefficient of non-uniformity of energy release at core fuel rods and 1.064 – maximum value of engineering coefficient of reserve for fuel rod power.
- The final value of the fraction of damaged rods claddings, and, accordingly, the fraction of the gas gap activity release, also takes into account the uneven energy release across the fuel rods of one assembly K_k (VVER design data for the fuel loads):
- o $K_k = K_r/K_q = 1.5/1.35 = 1.1111$ – VVER–1000 reactor core; $K_r = 1.5$ – maximum permissible coefficient of non-uniformity of energy release at core fuel rods and $K_q = 1.35$ – maximum permissible coefficient of non-uniformity of energy release by fuel assemblies;
- o $K_k = K_r/K_q = 1.62/1.46 = 1.1096$ – VVER–440 reactor core; $K_r = 1.62$ – maximum permissible coefficient of non-uniformity of energy release at core fuel rods and $K_q = 1.46$ – maximum permissible coefficient of non-uniformity of energy release by fuel assemblies;
- o the fraction F_{clad} of damaged fuel rods claddings of the assembly with a temperature above 800 °C (criterion ≥ 799.9 °C is adopted to cover the uncertainty) is determined by the limit of change in the unevenness of energy release across the fuel rods from $K_{k.low} = 1\text{-}(K_k\text{-}1) = 0.8889$ and 0.8904 to $K_{k.up} = K_k = 1.1111$ and 1.1096 (VVER–1000 and VVER–440 data); this fraction is calculated as $F_{clad}=(K_{k.up}\text{-}799.9/T_{max})/(K_{k.up}\text{-}K_{k.low})$, where T_{max} – maximum calculated temperature of claddings outer surface for individual HCO of core model for ATHLET code.

For LOCA scenarios the fractions F_{clad} of damaged fuel rods claddings according to thermomechanical criterion (which used for evaluation of fraction of the gas gap activity release) are as follows:

- VVER–1000/DBA, «CL guillotine break with a diameter of 2 × 850 mm» scenario – $F_{clad} = 29.355078/163 = 0.18009$; 163 – total number of fuel assemblies of VVER–1000 reactor core, 29.355078 – calculation value of the number of equivalent fuel assemblies for which the criterion for the temperature of the fuel rods claddings of 800 °C is violated;
- VVER–1000/DBA, «CL break with a diameter of 350 mm» – $F_{clad}=(1/312)/163 = 1.9663E–05$; 163 – total number of fuel assemblies of VVER–1000 reactor core, 1/312 – one fuel rod of one assembly for which the criterion for the temperature of the fuel rods claddings of 800 °C is violated (calculation value);
- VVER–1000/DEC–A, «CL guillotine break with a diameter of 2 × 850 mm» scenario – $F_{clad} = 9.52036/163 = 0.05841$; 163 – total number of fuel assemblies of VVER–1000 reactor core, 9.52036 – calculation value of the number of equivalent fuel assemblies for which the criterion for the temperature of the fuel rods claddings of 800 °C is violated;
- VVER–440/DBA, «CL guillotine break with a diameter of 2 × 500 mm» scenario – $F_{clad} = 1.0/(312 + 37) = 0.00287$; 312 – total number of fuel assemblies of VVER–440 reactor core (Unit 2 of the Rivne NPP), 37 – total number of fuel assemblies with control rods of VVER–440 reactor core (Unit 2 of the Rivne NPP), 1.0 – calculation value of the number of equivalent fuel assemblies for which the criterion for the temperature of the fuel rods claddings of 800 °C is violated.

Table 2 shows the main characteristics of the HCOs of the modified core model of the VVER-1000 and VVER-440 reactors, which is used at the stage of preliminary calculations to estimate the fraction of damaged fuel rods claddings and, accordingly, to estimate the fraction of gas gap activity release. Table 2 shows the coefficient of non-uniformity of energy release by fuel assemblies (K_q), the number of assemblies with the corresponding K_q and Thermal Fluid Objects (TFOs) of the core model, to which the HCOs corresponds. Some coefficients of unevenness of energy release K_q are slightly changed relative to the value in accordance with the fuel load cartogram (marked with the symbol "**" in the Table 2). This is necessary for setting the exact value of the reactor heat power, which is: 3120 and 3000 MW for VVER–1000 reactor at DBA and DEC–A conditions respectively; 1423.2 and 1375.0 MW for VVER–440 reactor at DBA and DEC–A conditions respectively. It should be noted that the data in Table 2 for the VVER–440 reactor are given only for DBA conditions, since the criterion temperature of 800 °C for damage to the claddings is not reached for all DEC–A scenarios.

2.2.3. Evaluation of the release of isotopes activity into the containment

The integral activity of the release of the i-th isotope from the primary circuit to the containment through the leak is calculated on the basis of the mass balance of the equivalent (boron) particles, which represent the isotopes. The isotopes release activity is determined by the ratio of the mass of these equivalent particles at the k-th time interval, which left the system of the primary circuit into the leakage, to the total initial or maximum mass of these particles in the core as follows:

- integral release of i-th isotopes activity into containment with leak:

$$A_{k.i} = N_{k.i} \times \lambda_i(Bq),$$

where $N_{k.i}$ – integral accumulated number of i^{th} released isotopes particles; λ_i – decay constant of i^{th} isotope (s^{-1}); the definition of λ_i is given in para.1.2.1 of this article;

- integral accumulated number of i^{th} isotopes particles released into containment:

$$N_{k.i} = [(A_i/\lambda_i)/N_{TOT.}] \times N_k,$$

N_k – accumulated number of all isotopes particles released into containment; $N_{TOT.} = SUM(A_{TOT.i}/\lambda_i)$ – total number of isotopes particles;

- integral accumulated number of all isotopes particles released into containment:

$$N_k = (N_{TOT.} \times M_{TOT.k})/M_{ISO.TOT},$$

where $M_{TOT.k}$ – released isotopes particles integral mass (kg); $M_{ISO.TOT}$ – maximum or total mass of nuclides into primary circuit system (kg); $N_{TOT.}$ – total number of isotopes particles.

The final release of isotopes activity into the environment is estimated by calculation using the containment model for the COCOSYS code.

Table 2
Main parameters of the HCOs of core model for VVER–1000 and VVER–440 fuel load at beginning of the fuel cycle.

VVER–1000				VVER–440				VVER–440 (data continuation)			
Item of HCOs	K_q	Fuel assemblies number	Core TFOs region	Item of HCOs	K_q	Fuel assemblies number	Core TFOs region	Item of HCOs	K_q	Fuel assemblies number	Core TFOs region
1	0.32	11	P*	1	0.22	17	AC*	31	1.25	9	AC*
2	0.33	1	P*	2	0.23	7	AC*	32	1.26	3	AC*
3	0.46	4	P*	3	0.26	4	AC*	33	1.27	1	AC*
4	0.47	2	P*	4	0.27	6	AC*	34	1.28	6	AC*
5	0.66	1	C*	5	0.28	2	AC*	35	1.31	11	AC*
6	0.69	4	C*	6	0.33	2	AC*	36	1.32	4	AC*
7	0.70	2	C*	7	0.34	4	AC*	37	1.33	3	AC*
8	0.89	6	C*	8	0.35	6	AC*	38	1.36	9	AC*
9	0.90	6	C*	9	0.45	5	AC*	39	1.37	10	AC*
10	0.92	4	P*	10	0.46	7	AC*	40	1.382	4	AC*
11	0.93	8	P*	11	0.62	14	AC*	41	1.39	8	AC*
12	0.97	6	C*	12	0.63	4	AC*	42	1.40	10	AC*
13	0.98	13	C*	13	0.65	12	AC*	43	1.411**	16	AC*
14	0.99	11	C*	14	1.01	1	AC*	44	1.422**	10	AC*
15	1.09	6	P*	15	1.03	19	AC*	45	1.432**	3	AC*
16	1.10	6	P*	16	1.04	17	AC*	46	1.44	1	AC*
17	1.11	1	P*	17	1.05	8	AC*	47	0.42	4	CR*
18	1.12	8	P*	18	1.06	14	AC*	48	0.43	2	AC*
19	1.12	2	C*	19	1.07	5	AC*	49	1.05	1	AC*
20	1.13	3	P*	20	1.08	2	AC*	50	1.15	8	AC*
21	1.13	4	C*	21	1.11	5	AC*	51	1.16	8	AC*
22	1.18	4	C*	22	1.12	6	AC*	52	1.17	2	AC*
23	1.19	8	C*	23	1.13	1	AC*	53	1.20	1	AC*
24	1.23 (DBA) 1,233** (DEC–A)	6	C*	24	1.14	6	AC*	54	1.21	4	AC*
25	1.24 (DBA) 1.241** (DEC–A)	16	C*	25	1.15	5	AC*	55	1.22	1	AC*
26	1.246** (DBA) 1.248** (DEC–A)	2	C*	26	1.16	1	AC*	56	1.27	1	AC*
27	1.26	7	C*	27	1.20	1	AC*	57	1.28	4	AC*
28	1.266** (DBA) 1.27 (DEC–A)	8	C*	28	1.21	11	AC*	58	1.29	1	AC*
29	1.28	2	C*	29	1.23	9	AC*	59	1.4892	125/126 = 0.992063	HA*
30	1.4175 (DBA) 1.35 (DEC–A)	311/312 = 0.996795	HA*	30	1.24	2	AC*	60	1.72368	1/126 = 0.007937	HR*
31	1.74 (DBA) 1.5 (DEC–A)	1/312 = 0.003205	HR*								

Note:
** – K_q, the values of which have been slightly changed in comparison with the core loading cartogram to maintain the required power of the reactor;
P* – peripheral core part;
C* – central core part;
AC* – average core;CR* – fuel assemblies with control rods (absorber of the VVER–440 core);
HA* – 311, 125 average rods of hot assembly for VVER–1000, VVER–440 respectively;
HR* – 1 hot rod of hot assembly.

3. Activity release from primary circuit into containment

The primary leaks from cold leg at reactor entrance to the containment with 2×850, 350, 100 and 50 mm diameters are simulated for the VVER-1000. LOCA scenarios with 2×500, 250, 100 and 50 mm diameters of leakage are simulated for the VVER-440. For DBA LOCA scenarios conservative assumptions (IAEA-EBP-WWER-01, 1995; IAEA. Vienna., 2002) are applied for both thermohydraulic and radiological consequences simulations. For DEC–A LOCA thermohydraulic simulations a realistic approach for initial conditions is adopted with nominal primary and secondary initial parameters (IAEA. Vienna., 2002), except for the application of maximum peaking factors for “hot” fuel assembly and “hot” fuel rod power distribution. Data on the initial and boundary conditions of the calculation scenarios are given in sections 2 and 3 of article (Berezhnyi et al., 2023). It should be noted that for a conservative calculation formulation in relation to the assessment of the radiological consequences of a the LOCA scenarios, which is given in article (Berezhnyi et al., 2023), and for a more realistic calculation formulation, which is considered in this article, the same set of initial and boundary conditions is considered. The difference of the improved methodology lies in more realistic modeling of the release and transport of radionuclides from the primary circuit system to the containment space through the CL rupture.

The calculation of the release of radionuclide activity from the primary circuit due to leakage into the containment is performed using the reactor coolant system model for the ATHLET3.2/AC[2] code (Lerchi et al., 2019; Austregesilo et al., 2019). Calculations were carried out on a time interval taking into account the completion of the FP release from the primary circuit and conditional stabilization of the state of the reactor unit.

Compared to the conservative approach (Berezhnyi et al., 2023), modelling improvements are focussed on evaluating of the phenomenology of the following processes:

- only the part of the activity of the gas gap is considered, which meets the accepted thermomechanical criteria for damage of the fuel rod claddings;
- the mechanism of transport of radionuclides from the primary circuit to the containment through the leak has been implemented;
- the dilution of radionuclides in primary circuit by supplying a «clean» coolant from passive and active ECCS is considered;
- deposition of radionuclides in the volumes of the primary circuit is taken into account, when the concentration of isotopes that exceeds the maximum solubility in the water coolant.

A conservative approach (Berezhnyi et al., 2023) to the assessment of the radiological consequences of the LOCAs assumes the release of gas gap content of all fuel rods, which happens during the time of leakage into the containment of coolant mass, which is equal to the initial primary circuit inventory, without taking into account dilution and deposition of isotopes. Improved modelling, especially due to taking into account the thermomechanical criterion of damage of the fuel claddings leads to a significant decrease in the release of radionuclides activity in the containment during the LOCAs.

Fig. 2 shows a comparison of the distribution over time of the integral release of the total activity of all isotopes from the primary circuit to the containment through the break during LOCA DBA and DEC-A scenarios. Brown graphs show conservative estimates, and blue graphs show the results of the improved calculation methodology.

Table 3 shows the grouped calculation results regarding the value of the integral release and the time duration of the release of the radionuclide activity from the primary circuit into the containment. The results are given for all scenarios, for reactor units with VVER–1000 and VVER–440 reactors, both for conservative and realistic calculation methodology. Table 3 also shows the value of the reduction in activity release due to improved modelling of radiological consequences of the LOCAs.

4. Activity release from containment to environment

Evaluation of the release of activity of radionuclides from containment into environment is performed using the containment model for the COCOSYS3.0 code (Arndt et al., 2020). Calculations were performed for a problem time of three days for VVER–1000 and one day for VVER–440 reactor units, respectively (72 and 24 h) – guaranteed time to ensure the safety and autonomy of the NPP with VVER-1000 and

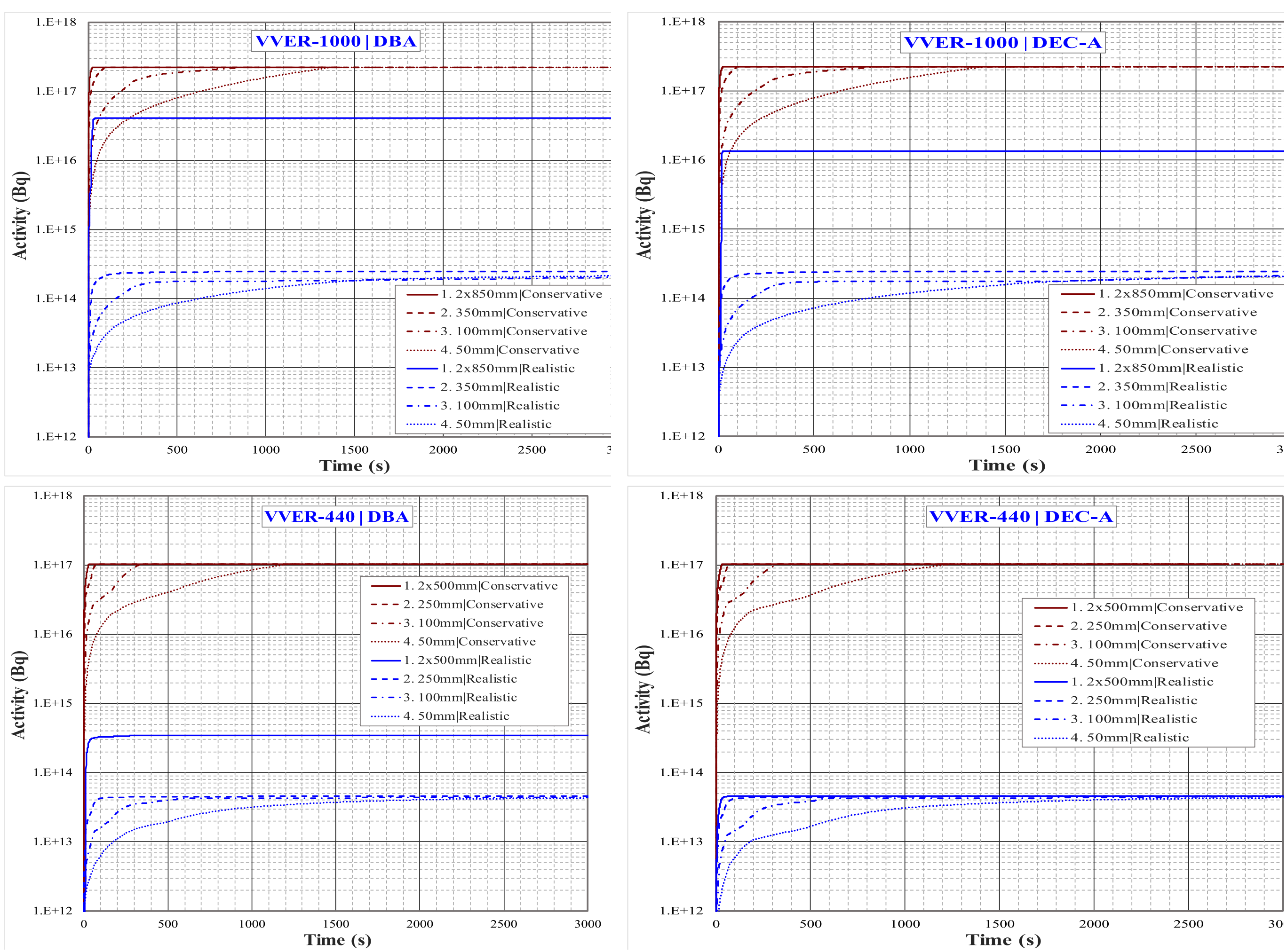

Fig. 2. Integral FP release from primary into containment for conservative and realistic calculation approaches.

Table 3
The comparison of FP release into the containment at conservative and improved calculation approaches.

Scenario of primary circuit leak	FP release into containment (Bq)		Time duration of activity release into containment (s)		Multiplicity of reduction of activity release into containment
	Conservative	Realistic	Conservative	Realistic	
VVER–1000 | LOCA DBA					
1. 2 × 850 mm	2.252E + 17	4.082E + 16	24	70	5.5
2. 350 mm	2.252E + 17	2.458E + 14	93	194	916
3. 100 mm	2.252E + 17	2.414E + 14	891	6244	933
4. 50 mm	2.252E + 17	2.414E + 14	1383	13,800	933
VVER–1000 | LOCA DEC–A					
1. 2 × 850 mm	2.252E + 17	1.340E + 16	24	73	16.8
2. 350 mm	2.252E + 17	2.414E + 14	98	316	933
3. 100 mm	2.252E + 17	2.414E + 14	855	8840	933
4. 50 mm	2.252E + 17	2.414E + 14	1401	13,000	933
VVER–440 | LOCA DBA					
1. 2 × 500 mm	1.039E + 17	3.437E + 14	30	236	302
2. 250 mm	1.039E + 17	4.599E + 13	75	1170	2259
3. 100 mm	1.039E + 17	4.599E + 13	350	5680	2259
4. 50 mm	1.039E + 17	4.599E + 13	1250	13,300	2259
VVER–440 | LOCA DEC–A					
1. 2 × 500 mm	1.039E + 17	4.599E + 13	34	82	2259
2. 250 mm	1.039E + 17	4.599E + 13	76	1620	2259
3. 100 mm	1.039E + 17	4.599E + 13	337	8050	2259
4. 50 mm	1.039E + 17	4.599E + 13	1270	13,550	2259

VVER–440 reactor respectively during emergency processes of the DBA and DEC-A type without intervention of operational personnel.

Calculation scenarios of processes in the containment at more realistic evaluation of radiological consequences are based on new inputs data obtained using the ATHLET reactor coolant system model, which takes into account a partition damage of the fuel rods claddings with the corresponding portion of release of gas gap content and detailed calculations of the isotopes transport from the primary circuit through the break. It should also be noted that within the conservative approach to the safety analysis of Ukrainian NPPs for both DBA and DEC-A scenarios, the containment model for the COCOSYS code (for VVER–1000 and VVER–440) does not consider the operation of the Filtered Containment Venting System (FCVS). The functioning of the FCVS is considered within the long-term management of severe accidents in order to reduce the radiological consequences of such accidents. Severe accidents are not considered in this calculation study.

The computational analysis of the processes in the containment with using the COCOSYS model related to the phenomenology of the primary circuit leakage was performed on the basis of the following boundary conditions from the ATHLET model:

- time distribution of concentration or specific mass flow of isotopes that pass from the primary circuit to the containment through the rupture. For the COCOSYS code groups of isotopes based on 8 chemical elements (krypton Kr, xenon Xe, strontium Sr, rubidium Ru, iodine I, caesium Cs, lanthanum La and cerium Ce) are considered, that is, the characteristics of all isotopes within one element are summed up for them;
- time distribution of mass flow rate and enthalpy of the liquid and vapour phase of the leakage flow. Identical boundary conditions for conservative and realistic calculation approach;
- time distribution of mass flow rate of the coolant injection into primary circuit from high and low pressure injection systems. Identical boundary conditions for conservative and realistic calculation approach.

Modified calculation scenarios for the COCOSYS model involve considering a more detailed particle size classes spectrum – more detailed and realistic modelling of the isotopes transport within the containment. The modified calculation analysis due to improved modelling of the behaviour of radionuclides ensures a significant reduction of the radiological consequences of the LOCAs in comparison with a conservative approach. Fig. 3 shows a comparison of the time distribution of the integral release of the total activity of all isotopes from the containment to the environment during LOCA DBA and DEC-A scenarios. Brown graphs show conservative estimates, and blue graphs show the results of the improved calculation methodology.

Table 4 shows the grouped calculation results regarding the value of the integral release of radionuclide activity into the environment. Relative distribution of the activity release by groups of radionuclides at the time of completion of the calculation analysis is shown. Chemically inert and light isotopes of noble gases, such as Xe and Kr, are emitted into the environment with liquid, vapour and air phases due to the looseness of the containment throughout the emergency process, therefore their faction is the largest. The value of the reduction in activity release due to the improved modelling is also given.

As can be seen from the Table 4 and Fig. 3, for the scenario of 250 mm break for the VVER–440 reactor unit, slightly larger values of the release of activity into the environment are observed in comparison with the scenario with the maximum size of the primary circuit leakage (2 × 500 mm) for conservative calculation. Such results are associated with an increase in the fraction of the iodine isotopes release into the environment for scenario with a leakage size of 250 mm due to a decrease in the efficiency of isotope capture by the passive condenser of the VVER–440 reactor unit with a lower flow of coolant into the leakage. Iodine isotopes have the greatest activity in the primary circuit. With a realistic approach to the analysis, due to taking into account the thermomechanical criterion of damage to the fuel rod claddings, the radiological consequences for all cases are correlated with the leakage size of the primary circuit.

5. Radiological consequences evaluation

The environmental dose calculation were performed using the tool (Olivier, 2022) developed in the framework of R2CA project by TRACTEBEL ENGINEERING S.A.

The height of the release point corresponded to the lowest NPP outside constructions elevation (0 m) which according to the methodology (Olivier, 2022) is 1 m, that is, it is the lower starting point of the calculation methodology in relation to the radioactive emission elevation. This approach corresponds to the generally accepted methodology for assessing the radiation consequences of the LOCAs type, if the methodology itself does not take into account the absorbing effect of the earth's litter, which corresponds to the used simplified methodology. And also the doses were determined for a distance of 2.5 km from the NPP – as for VVER–1000 and for VVER–400 reactor units. Thyroid equivalent doses are calculated regarding to the methodology (Olivier, 2022), and effective doses, which are subject to regulatory requirements, obtained taking into account the weight coefficient of

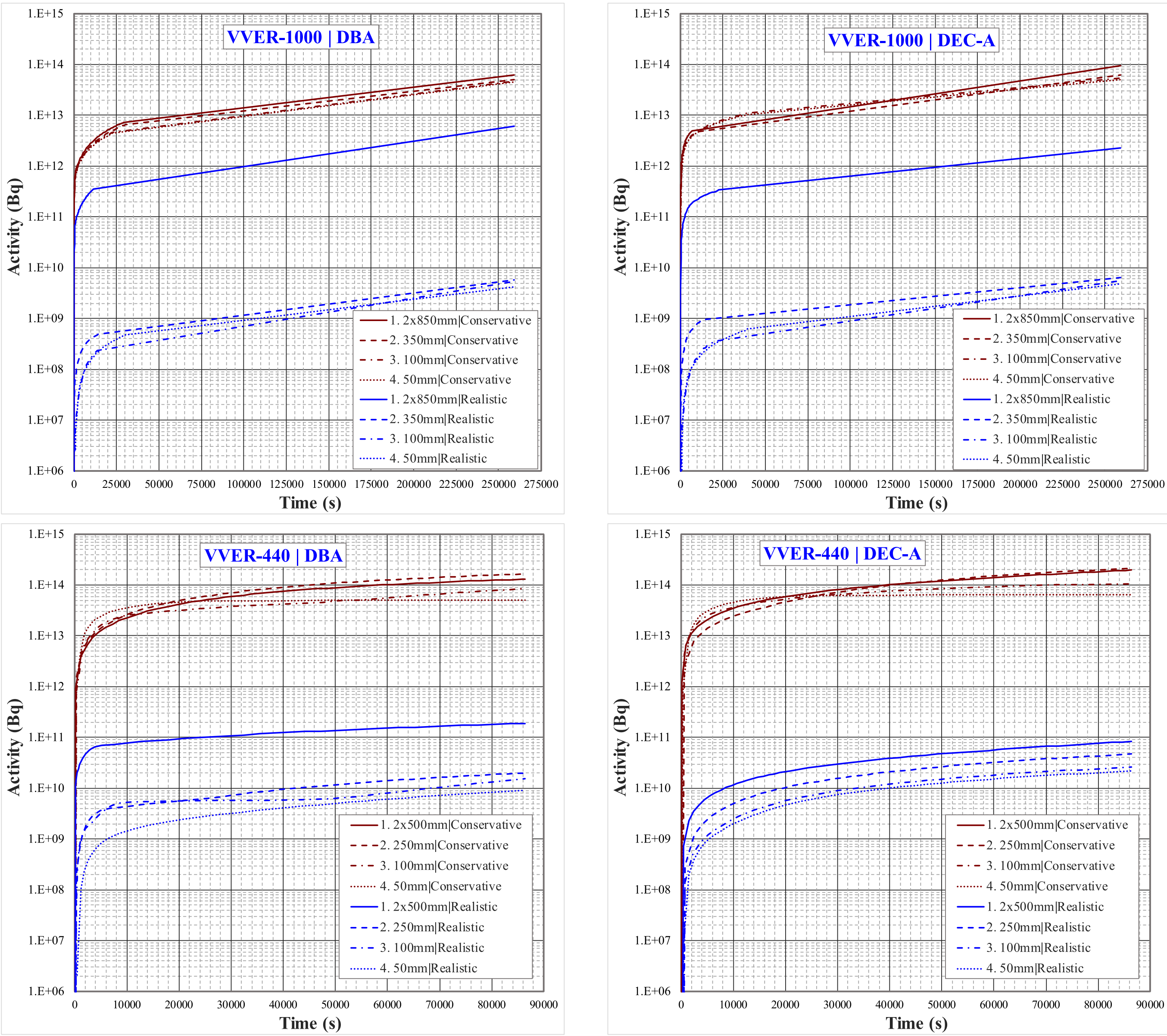

Fig. 3. Integral FP release from containment to environment for conservative and realistic calculation approaches.

radiation for the thyroid, which is 0.05.

Table 5 shows the grouped calculation results regarding the maximum value of the radiological consequences for all scenarios, namely maximum value of the thyroid and total effective doses among population ages groups. Table 5 also shows the value of the reduction in maximum effective dose due to improved modelling of radiological consequences of the LOCA incidents. As can be seen from the Table 5, the application of the improved modelling with more realistic isotopes behaviour leads to a very significant reduction of the radiological consequences of the analysed accidents of LOCA type.

6. Conclusions

In the practice of deterministic safety analysis with regard to the radiological consequences of the LOCA emergency events, both of the DBA and DEC–A categories for reactor units VVER–1000 and 440, a conservative approach is applied. This paper proposes an improved methodology for more realistic modelling of radiological consequences compared to a conservative approach.

Regarding to the reduction of the LOCA radiological consequences, improvements in modelling are provided by considering the followings:

- approved thermomechanical criteria are considered in relation to the damage of the fuel rod claddings with the subsequent release of the portion of the gas gap activity content;
- transport of radionuclides from the primary circuit to the containment through the leak is implemented;
- dilution of radionuclides by supplying non-radioactive coolant from the passive and active ECCS is considered;
- deposition of radionuclides in the volumes of the primary circuit is taken into account, when the concentration of isotopes that exceeds the maximum solubility in the water coolant;
- more detailed and realistic modelling of the isotopes transport within the containment is performed.

A simplified conservative assessment of the radiological consequences of the LOCAs (Berezhnyi et al., 2023) assumed the release into containment of all activity of isotopes in the primary circuit system for all scenarios. The improved approach involves modelling the behaviour of isotopes in the primary circuit system with equivalent particles of

Table 4
The comparison of FP release into the containment at conservative and improved calculation approaches.

Scenario of primary circuit leak	FP release to environment (Bq)		Distribution of the portion of FP release to the environment by isotopes groups (%)								Reduction of FP release to environment
	Conservative	Realistic	Kr	Xe	Sr	Ru	I	Cs	Ce	La	
VVER–1000 | LOCA DBA											
1. 2 × 850 mm	6.194E + 13	6.211E + 12	9.603	89.29	0.018	0.127	0.205	0.047	0.474	0.237	10
2. 350 mm	5.002E + 13	5.700E + 09	0.626	98.172	9.E–04	6.E–04	1.154	0.010	0.025	0.012	8776
3. 100 mm	4.734E + 13	5.312E + 09	0.498	98.535	1.E–07	2.E–07	0.961	0.006	4.E–07	1.E–05	8911
4. 50 mm	4.592E + 13	4.241E + 09	0.257	98.739	1.E–07	2.E–07	0.997	0.007	4.E–07	1.E–05	10,827
VVER–1000 | LOCA DEC–A											
1. 2 × 850 mm	9.403E + 13	2.283E + 12	8.043	82.660	0.143	1.019	1.840	0.381	4.029	1.886	41
2. 350 mm	6.300E + 13	6.392E + 09	0.423	86.462	5.E–06	1.E–05	13.013	0.102	1.E–05	2.E–04	9855
3. 100 mm	5.403E + 13	5.594E + 09	0.247	93.753	9.E–07	1.E–06	5.958	0.042	3.E–06	7.E–05	9659
4. 50 mm	5.111E + 13	4.808E + 09	0.253	98.015	5.E–07	7.E–07	1.721	0.011	1.E–06	2.E–05	10,632
VVER–440 | LOCA DBA											
1. 2 × 500 mm	1.31E + 14	1.90E + 11	3.406	87.266	0.125	0.884	2.547	0.421	3.256	2.095	687
2. 250 mm	1.66E + 14	2.00E + 10	0.511	96.489	1.E–05	9.E–05	2.968	0.031	3.E–04	7.E–04	8300
3. 100 mm	8.50E + 13	1.52E + 10	0.474	96.714	9.E–06	1.E–05	2.788	0.024	3.E–05	8.E–05	5592
4. 50 mm	5.10E + 13	9.10E + 09	0.430	96.748	1.E–06	6.E–06	2.802	0.020	4.E–06	1.E–05	5604
VVER–440 | LOCA DEC–A											
1. 2 × 500 mm	1.98E + 14	8.39E + 10	3.631	92.051	0.098	0.745	2.158	0.218	0.916	0.183	2360
2. 250 mm	2.14E + 14	4.70E + 10	0.629	96.113	1.E–05	9.E–05	3.237	0.021	1.E–04	2.E–04	4553
3. 100 mm	1.07E + 14	2.60E + 10	0.602	96.745	6.E–07	9.E–07	2.634	0.019	1.E–05	4.E–05	4115
4. 50 mm	6.50E + 13	2.17E + 10	0.558	96.761	4.E–07	9.E–07	2.663	0.018	1.E–06	5.E–05	2995

Table 5
Maximum value of the thyroid and total effective doses among population ages groups.

Leak diameter (mm)	Max thyroid effective doses (mSv)		Max total effective doses (mSv)		Reduction of max thyroid dose	Reduction of max total dose
	Conservative	Realistic	Conservative	Realistic		
VVER–1000 | LOCA DBA						
2 × 850	3.97E-02	3.96E-03	3.45E-01	3.46E-02	10	10
350	1.72E-01	1.94E-05	1.06E-01	1.23E-05	8866	8618
100	1.35E-01	1.14E-05	7.39E-02	6.34E-06	11,842	11,656
50	1.34E-01	8.90E-06	7.32E-02	4.98E-06	15,056	14,699
VVER–1000 | LOCA DEC–A						
2 × 850	5.40E-01	1.28E-02	4.37E + 00	1.06E-01	42	41
350	1.84E + 00	1.82E-04	9.97E-01	9.90E-05	10,110	10,071
100	6.62E-01	6.71E-05	3.59E-01	3.64E-05	9866	9863
50	1.97E-01	1.82E-05	1.08E-01	9.96E-06	10,824	10,843
VVER–440 | LOCA DBA						
2 × 500	4.51E-01	5.82E-04	2.38E + 00	3.41E-03	775	698
250	6.31E-01	6.71E-05	4.31E-01	4.38E-05	9404	9840
100	4.80E-01	5.65E-05	3.26E-01	3.67E-05	8496	8883
50	2.89E-01	3.40E-05	1.99E-01	2.17E-05	8500	9171
VVER–440 | LOCA DEC–A						
2 × 500	5.71E-01	1.75E-04	1.57E + 00	3.87E-04	3263	4057
250	8.87E-01	1.41E-04	5.98E-01	7.74E-05	6291	7726
100	5.71E-01	1.01E-04	3.88E-01	5.48E-05	5653	7080
50	3.51E-01	8.50E-05	2.41E-01	4.63E-05	4129	5205

boric acid of a certain concentration, which corresponds to the number of radionuclide particles or their activity, using the ATLET model.

The most significant impact on the reduction of radiological consequences of the LOCAs has the consideration of the phenomenology of damage to the fuel rods claddings and the corresponding more realistic assessment of the fraction of the activity release of the fuel rods gas gap. The improved modelling considers a detailed model of the core heat structures, which takes into account the entire spectrum of unevenness of energy release in fuel assemblies and allows for a detailed assessment of the portion of fuel rods for which the condition of claddings damage is reached at a temperature of the outer surface of the claddings above 800 °C. Thus, for the most significant scenario with regard to radiological consequences, namely, a rupture with an equivalent diameter of 2 × 850 mm for a VVER–1000 reactor unit of the DBA category, a significant reduction of the dose load by approximately 10 times is achieved. For other scenarios, a much larger dose reduction of about 2–4 orders of magnitude is achieved due to the absence of conditions for the release of gas gap activity for most scenarios (see Table 5).

Detailed modelling of the transport and dilution of isotopes in the primary circuit system on the way to the leakage of the coolant into the containment also significantly affects the reduction of the radiological consequences of the LOCAs. For example, for the most significant scenario of «2 × 850 mm break, VVER–1000, DBA», the reduction in the activity of the isotopes release from the primary circuit to the containment is about 5.5 times (see Table 3) due to taking into account the thermomechanical criterion of damage to the fuel rods claddings. Reduction of the FP release to the environment and the dose effects is about 10 times (see Table 4 and Table 5) due to a more realistic distribution in time of the concentration of radionuclide particles in the coolant.

As a result of the significant dynamics of losses of the primary coolant through the break and their effective mixing for all considered scenarios of the LOCAs, the influence of the solubility of isotopes in the coolant, namely the deposition of radionuclide particles, is insignificant in relation to the release of activity into the containment. The deposition of radionuclides in the volumes of the primary circuit increases the final release time of all activity in the containment by approximately 2–10 %, which practically does not affect the resulting radioactive consequences to the environment.

Considering a detailed particle size classes spectrum in the COCOSYS containment model provides more realistic modelling of the isotopes transport within the containment. The reduction of radiological consequences (dose burden) due to this improvement in modelling is relatively insignificant and amounts to about 2–4 % for various scenarios.

In general, the improved calculation approaches considered in this paper provide a significant reduction in the conservatism of the assessment of the radiological consequences of the LOCAs scenarios. That is, such improved modelling provides a more realistic estimates of the dose burden to the public. Further studies to improve and increase the accuracy of the assessment of the radiological consequences of the LOCAs relate to can be focused on the following aspects:

- assessment of a more realistic isotopic composition in the primary circuit system, both in relation to the radionuclides dissolved in the coolant and the spike effect at the beginning of the emergency process, and in relation to the isotopic composition of the gas gap content of the fuel rods;
- study of the influence of a more detailed model not only of the core heat structures (in relation to the unevenness of the energy release), but also of the core hydrodynamic elements in relation to the unevenness of the coolant flow distribution through the fuel assemblies;
- analytical and calculation assessment of the degree of deposition and chemical transformations in the system of the primary circuit and containment of the most significant dose-forming radionuclides, such as iodine isotopes.

CRediT authorship contribution statement

A. Berezhnyi: Writing – review & editing, Data curation, Conceptualization. **A. Krushynskyy:** Writing – review & editing, Data curation, Conceptualization. **D. Ruban:** Writing – original draft, Visualization, Methodology, Investigation, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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