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AURIMAS KONTAUTAS

# **The Numerical Study of Aerosol and Radionuclide Transport in the Containments of Nuclear Power Plants**

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Summary of Doctoral Dissertation  
Technological Sciences, Energetics and Power Engineering (06T)  
2013, Kaunas

KAUNAS UNIVERSITY OF TECHNOLOGY  
LITHUANIAN ENERGY INSTITUTE

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PLANTS**

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KAUNO TECHNOLOGIJOS UNIVERSITETAS  
LIETUVOS ENERGETIKOS INSTITUTAS

AURIMAS KONTAUTAS

**AEROZOLIŲ IR RADIONUKLIDŲ PERNAŠOS BRANDUOLINIŲ  
JĖGAINIŲ APSAUGINIUOSE KIAUTUOSE SKAITINIS TYRIMAS**

Daktaro disertacijos santrauka

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## **Introduction**

The operation of nuclear power plants (NPP) is related with a risk of loss of coolant accident, which could lead to release of radioactive materials to the environment. In order to prevent spread of radioactive material outside the power plant it is necessary to understand the processes that occur during accidents in nuclear power plants.

Most of radioactive materials that can escape from a nuclear power plant during a severe reactor accident will do so in the form of aerosol. Aerosol are very small solid particles or liquid droplets suspended in a gas phase. The suspended solid or liquid particles typically have a range of size. Particles may range in size from 0.01  $\mu\text{m}$  to 100  $\mu\text{m}$  [1]. The last barrier in the nuclear power plant, which prevents the radioactive material from release to the environment, is containment. The containment is a cylindrical reinforced structure, which enshrouds the piping of the reactor cooling system and the reactor itself. Due to the crack of the piping of reactor cooling system the contaminated by radioactivity coolant flow drains into containment, in which radioactive materials must be maintained until it will be pointed to cleaning systems or its activity decreases due to natural processes of radioactive decay.

A distribution of aerosol and radionuclides in nuclear power plant containments is studied for a long time. Various experimental and numerical research programmes (DEMONA, KAEVER, OECD-THAI, PHEBUS) were developed for the analysis of these processes. The lumped-parameter codes (COCOSYS, ASTEC, MELCOR, CONTAIN and others) are usually used for numerical studies in containment atmosphere. Nowadays codes are more advanced than 20 years ago, but an integrated methodology, which could validate usage of these codes for the aerosol and radionuclides transportation in containment atmosphere, has not been created.

The numerical study of aerosol and radionuclides transport processes using PHEBUS FPT-1 and FPT-2 experiment results was accomplished in this work. Also the parametrical analysis of deposition velocity and distribution was carried out. Suggestions were proposed for COCOSYS code improvement and for development of numerical model, which is used for this study of aerosol and radionuclides transportation processes.

### **The object of the Doctoral Dissertation**

Transport of aerosol and radionuclides in containments of water-cooled reactors.

### **The aim of the Doctoral Dissertation**

To justify the application of lumped-parameter approach in computer codes for the analysis of aerosol and radionuclides transport in the containments of nuclear power plants.

## **Tasks of the Doctoral Dissertation**

1. To investigate the influence of nodalisation of the containment formation on aerosol and radionuclide deposition processes.
2. To investigate the influence of various parameters (density, solubility factor, diffusive boundary layer) on aerosol and radionuclide deposition processes in containment.
3. To perform uncertainty and sensitivity analysis of the obtained results in order to evaluate the influence of parameters for aerosol and radionuclide deposition processes.
4. To prepare recommendations for development of a selected computer code and for the setting-up of numerical models.

## **Actuality of the Doctoral Dissertation**

Experimental studies of aerosol and radionuclide transport processes in containment are complex and expensive, so they could be changed or replaced by numerical studies, which are used for analysis of aerosol and radionuclide transport processes during normal exploitation or severe accidents. Numerical model, presented in this study, is designed for analysis of aerosol and radionuclide transport processes in light water reactor containments. Numerical results received with created model are in good agreement with PHEBUS international program experimental results. Recommendations for the setting-up of numerical model are presented.

## **Scientific novelty**

The application of lumped-parameter code COCOSYS for the analysis of aerosol and radionuclide transport processes in containments of nuclear power plant is confirmed.

## **Practical value**

Results of investigations renew COCOSYS code validation matrix.

Further, model could be successfully used for iodine chemistry processes investigation.

The recommendations for program code development and for setting-up of numerical mode offered in this work.

## **Statements carried out for defensive**

1. Internal convective flow rates must to be evaluated during the creation of numerical model.
2. The carried out investigation of PHEBUS FPT-1 and FPT-2 experiments revealed that the parameters (density of aerosols, the coefficient of solubility and the thickness of diffusion's layer) have only insignificant impact on the transport of aerosol and radionuclides.

3. The most significant influence on suspended aerosol mass deposition has dynamic shape factor.
4. The theory of Landau and Levich (ASTEC code), which enables to evaluate the heterogeneous structure of the boundary layer, is more suitable for investigation of aerosol deposition on boundary layer comparing with Prandtl and Taylor theory (COCOSYS code) in which turbulent flow is completely suppressed in boundary layer.

### **The structure and the content of the dissertation**

The dissertation consists of the following chapters: introduction, literature review, methodology, results, conclusions and references. General information on the content of dissertation is as follows: 106 pages, 73 figures, 13 tables and 81 references.

## **CONTENT OF THE THESIS**

### **1. REVIEW OF AEROSOL AND RADIONUCLIDES TRANSPORT PROCESSES IN CONTAINMENTS**

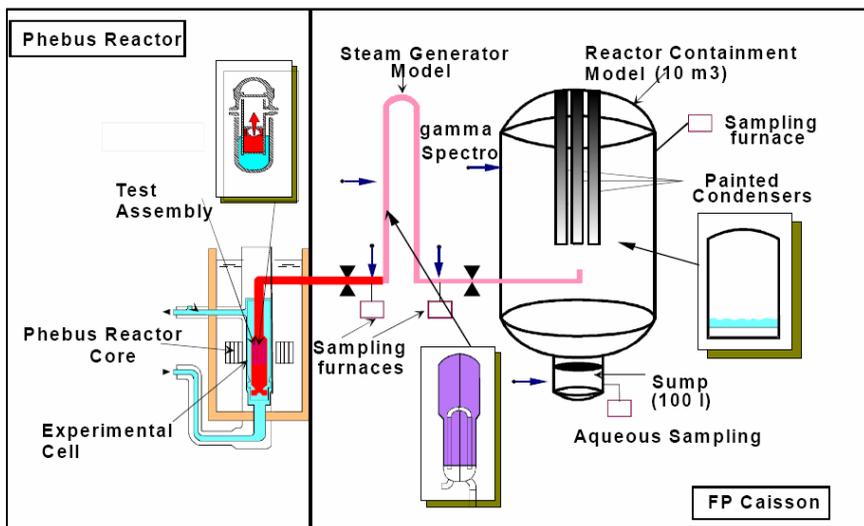
Most radioactive materials that can escape from a nuclear power plant during a severe reactor accident will do so in the form of aerosol. Aerosol mixed with steam flow could be transported through primary circuit, steam generator into containment atmosphere, where must be restrained and pointed to cleaning systems. Experimental and numerical analysis are performed to investigate aerosol and radionuclide transportation processes. Numerical investigations are required for interpretation and completing experimental results. Special program codes are used for numerical investigations, which permanently must to be verified. Aerosol transport and deposition comprehensive experimental investigations were performed in Battelle (Germany) research center. Containment named by DEMONA, in Battelle research center, with volume of 640 m<sup>3</sup> are mostly build in Germany pressurized water reactors (PWR). DEMONA [2] experiments were performed to investigate processes of aerosol transport and deposition by using tin oxide, iron oxide, silver and mixtures of chemicals at different thermal-hydraulic conditions. During VANAM [3] experiments the behaviour of aerosol in containment with different thermal-hydraulic conditions was analysed. KAEVER experimental facility can be equate to small experimental facilities, as compared with the DEMONA and VANAM, as it is only the volume of 10 m<sup>3</sup>. KAEVER experimental facility is also in Battelle research center in Germany. Main purpose of the KAEVER experiments was to investigate aerosol deposition processes in containment by using soluble (CSl, CsOH) and insoluble (Ag, SnO<sub>2</sub>) aerosol and their mixtures [4]. PHEBUS experimental and numerical research program began in 1988, after the events in the United States of America (Three Mile Island) in 1979 and in Ukraine (Chernobyl) in 1986 [5]. PHEBUS experimental facility is located in Cadarache

research center in France. The main objective of the program is to study the release, transport and retention of radionuclide in an in-pile facility under conditions representative of a severe accident in a Light Water Reactor (LWR).

Taking advantage from the results of the experiments were developed and validated FIPLOC [6], NAUA [7], CONTAIN [8], MELCOR [9], GOTHIC-MAEROS [10], ASTEC-CPA [11], COCOSYS [12] and other codes are used for the containment thermal-hydraulic, aerosol and radionuclide transport analysis. It was determined that by simulating aerosol and radionuclide transport processes it is necessary to estimate the fact that in containment, composed of a number of rooms, significant aerosol concentration differences, which determine the atmospheric stratification, could originate in these studies. In order to assess the flow patterns of gases it is important to compose certain detail nodalisation. The deposition of aerosol and radionuclides also strongly depends on other parameters such as hygroscopicity of material, relative humidity in the containment, which also have to be investigated. Program codes, evaluating the processes of transport and definition of aerosol and radionuclide, are tightly related with thermal-hydraulic parameters: pressure, temperature, relative humidity, atmospheric flows, leaks from containment and others. Variation of aerosol particles for the agglomeration, their deposition on the walls and their transport strongly depend on the following parameters in many aspects, therefore the objective evaluation of thermal-hydraulic processes is necessary at the beginning of the simulation of aerosol and radionuclide transport.

The numerical study of aerosol and radionuclide transport in PHEBUS containment with lumped-parameter code COCOSYS was performed in this work. PHEBUS experimental and numerical research program was implemented in Cadarache research centre in France in 1988 after major severe accidents in nuclear reactors at Three Mile Island (TMI, USA) in 1979 and at Chernobyl (Ukraine) in 1986. Common PHEBUS experiment technological scheme is shown in Figure 1. The diagram shows that the experimental stand is composed of three main components: active part, outline of reactor cooling system and containment.

PHEBUS is an international project, undertaken with the aim of evaluating the behaviour of radioactive fission products, released from a LWR pressure vessel into the containment vessel during a hypothetical severe accident. The facility provides prototypic reactor conditions. Those conditions enable to study the basic phenomena, which hold the release, transport, deposition and retention of the fission products. The studied phenomena came to pass in the core area, in the primary system components and in the containment building. The processes involved in these studies were thermal-hydraulics, physics, chemistry and radioactivity, which are closely coherent [14].



**Figure 1** PHEBUS facility technological view [13]

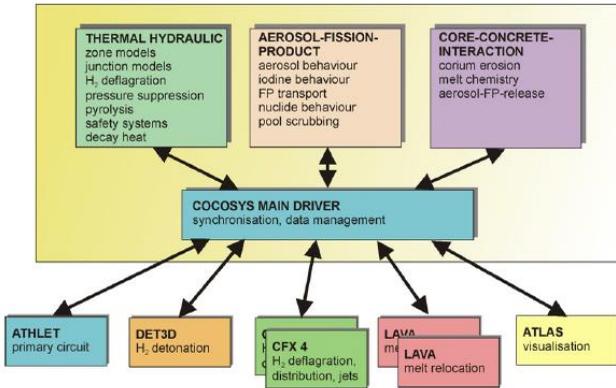
The Lithuanian Energy Institute has had a joined PHEBUS program since 2005. The most efforts of institute scientists were directed to investigation of containment phenomena using lumped parameter code COCOSYS. COCOSYS (Containment Code System) provides a code system on the basis of mechanistic models for the comprehensive simulation of all relevant processes and plant states during severe accidents in the containments of light water reactors and also covers the design basis accidents [12].

## **2. THE METHODOLOGY OF AEROSOL AND RADIONUCLIDES TRANSPORT PROCESSES IN CONTAINMENTS**

### **2.1. COCOSYS lumped-parameter program code**

The methodology of ongoing aerosol and radionuclides transport processes in PHEBUS containment is made by using the COCOSYS (Containment Code System) program code. This software package is under development and validation by GRS mbH (Germany) scientists on the base of CONTAIN, FIPLOC codes. These software packages were used for DEMONA, VANAM, KAEVER and other numerical studies. COCOSYS is a lumped-parameter program code designed for simulation of essential processes and states during severe accident propagation in the containment of light water reactors [12]. Program package is continuously verified on the basis of experimental data. COCOSYS is being used for the identification of possible deficits in plant safety, qualification of the safety reserves of the entire system, assessment of damage-

limiting or mitigating accident management measures. The complete system is divided into several so-called main modules (Figure 2).

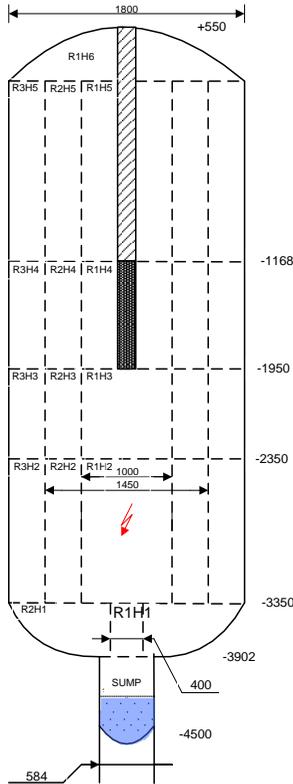


**Figure 2** Collaborating modules in COCOSYS system [12]

The COCOSYS has three main modules: thermo-hydraulics, aerosol and fission products and interaction of melt fuel with concrete. In addition to these main modules, which are part of the internal structure of the COCOSYS system, it is possible to plug in additional modules: ATHLET module – designed for simulation of processes in cooling system of reactor and for processes of fuel melting. DET3D and CFX4 are designed for modelling processes of combustion and explosion in the containment at the time of hydrogen emission. LAVA-designed for the modelling of the ongoing processes during the melting of fuel. ATLAS can be used for visualization of processes.

## 2.2. Model of PHEBUS containment

For simulation of aerosol and fission product transport in the PHEBUS containment model of 16 nodes was developed using COCOSYS code (see Figure 3). The radial subdivision consists of two rings, which are above the sump on the near level. There is a centre node R1H1 and node R2H1 that simulate the bottom part of the vessel. In level above -3350 mm and below 0 mm there are three almost equal area rings. The diameter of the radial subdivision was defined in such way that the flow areas in vertical direction are similar. Such approach gives similar gas flow velocities. A ring close to the external containment walls is 175 mm width. At the top vault of the vessel there is one additional node. Simulation at the top vault by single node gives the well-mixed conditions at the top of facility. Similar approach is used at the bottom of facility. Above the SUMP nodes are defined in such way that there are two junctions to the SUMP. Such approach ensures better mixing and allows avoiding dead-end node.



**Figure 3** Nodalisation scheme of PHEBUS containment

In the model there are defined 11 structures for the simulation of heat transfer through the containment walls to the outer atmosphere and 2 structures for the simulation of heat transfer between condensers and inner atmosphere. All PHEBUS containment surfaces and condensers are made of stainless steel and covered with epoxy paint. The characteristics of materials used for definition of structures have been described in experimental final report [15].

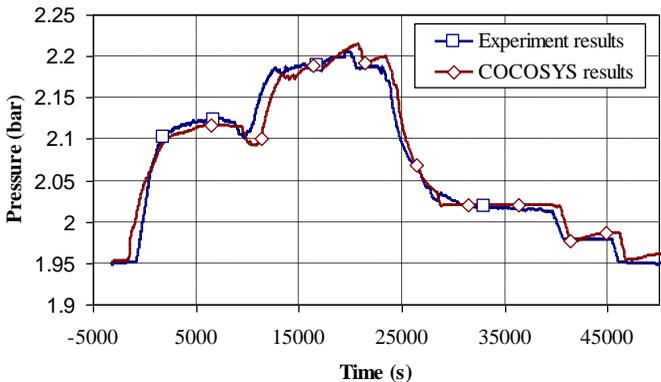
For the simulation of the gas flows between the nodes there are defined atmospheric junctions with real geometric areas. Also, there are defined junctions for simulation of the water drainage from the “wet” condenser to the sump. In the developed model the initial and boundary conditions (e.g. initial pressure, temperature, humidity, etc) are defined according to FPT-2 final report [15]. The initial pressure is 1.95 bar, initial average temperature is 108 °C and initial relative humidity is 51.29%.

The aerosol are divided into 20 size classes with the assumption that aerosol diameter is in range from  $10^{-8}$  to  $10^{-4}$  m. The gravitational, diffusive, diffusiophoretic, and thermophoretic deposition mechanisms are considered in the model. It is assumed that aerosol could be washed down from the vertical walls by condensate flow. The steam condensation on aerosol and slip through the vertical junctions is considered as well. Aerosol particles are assumed to be spherical and this assumption corresponds with the measured results. The thickness of diffusive boundary layer in PHEBUS containment is assumed  $10^{-4}$  m [16]. The soluble (Cs, Rb and I) and non-soluble (Ce, Te, Zr, Ru, Sn, In, Ag, W, U, Ba, Mo, Cd, Re and Tc) aerosol are defined in the model as separate aerosol components. The composition of elements detected in containment is given in FPT-2 Final test report [15]. It was estimated that the solubility factor for soluble elements is 1.73 and for non-soluble is 1.0.

### 3. RESULTS OF ANALYSIS

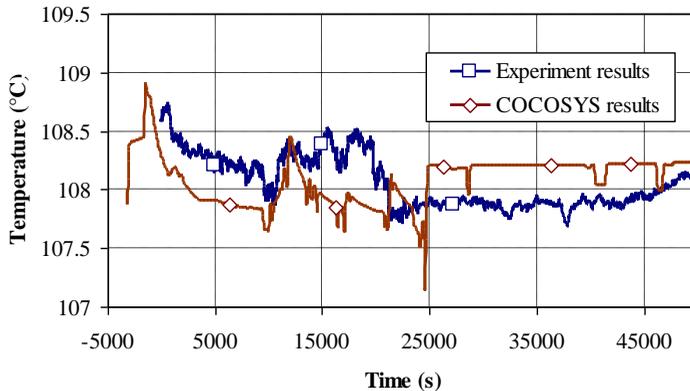
#### 3.1. Analysis of thermal-hydraulic parameters

The correct simulation of thermal-hydraulic phenomena is a precondition for simulation of transport and deposition of the aerosol and fission products in the containment. Comparison of calculated and measured total pressure is presented in Figure 4. At the beginning of the test transient, the steam injection of  $\sim 0.5$  g/s resulted in pressure increased from initial 1.95 bar to about 2.2 bar in 20000 s. Because of fuel cladding oxidation and consequently decrease of steam flow rate in time of 10000 s a sharp pressure decreased to 2.1 bar. After the containment was isolated, the pressure in experiment dropped to an initial value of  $\sim 1.95$  bar. There is only insignificant difference between calculated and measured pressure during the whole test sequence. The maximal total pressure was overestimated after 45000 s, but it was less then  $\sim 0.05$  bar, which is  $\sim 2\%$  of gauge pressure.



**Figure 4** Pressure in containment atmosphere

The comparison of calculated and measured gas temperature in the containment is presented in Figure 5. In general, the gas temperature evolution was predicted well and the difference between calculated and measured temperatures did not exceed 1 °C. After the containment isolation and sampling sequence the average measured and calculated gas temperature stabilized at the value close to 108 °C.

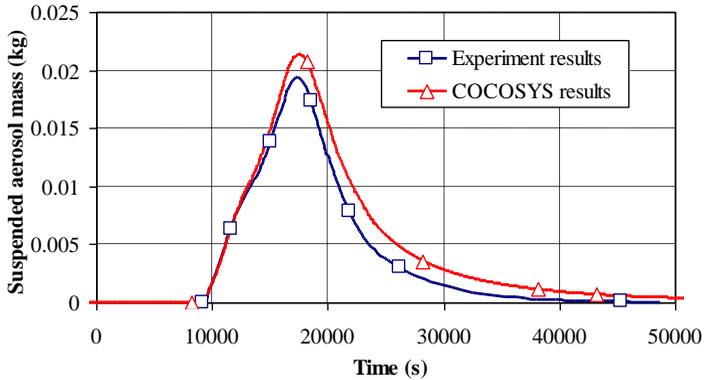


**Figure 5** Temperature in containment atmosphere

Taking into account the main thermal-hydraulic results (pressure and temperature) presented in Figure 4 and Figure 5, during FPT-2 in PHEBUS containment the thermal-hydraulic results were calculated quite well and there were no significant differences between the measured and calculated values. Such compliance reveals that the thermal-hydraulic part of containment model was developed to acceptable level and enables further analysis of aerosol and fission product transport and deposition processes, which is presented in the following sections.

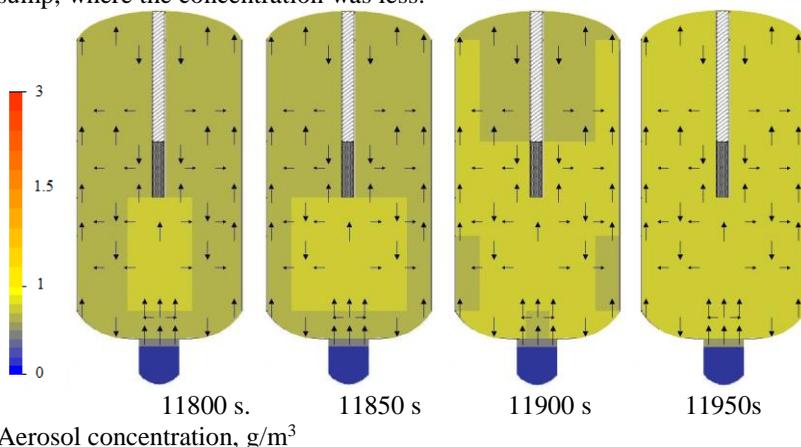
### 3.2. Analysis of aerosol transport in PHEBUS containment

Figure 6 presents a comparison between the measured and calculated aerosol mass suspended in the containment atmosphere. Aerosol injection to containment started after 9100 s and after ~17600 s was observed a maximum of the suspended airborne aerosol mass. In general the calculated airborne aerosol mass was overestimated during whole analyzed period, but the difference was less than 2 g. The maximal measured mass was ~19 g, while calculated was ~21 g. The difference between the calculated and measured mass does not change significantly, which shows that the deposition rate is rather well calculated by COCOSYS.



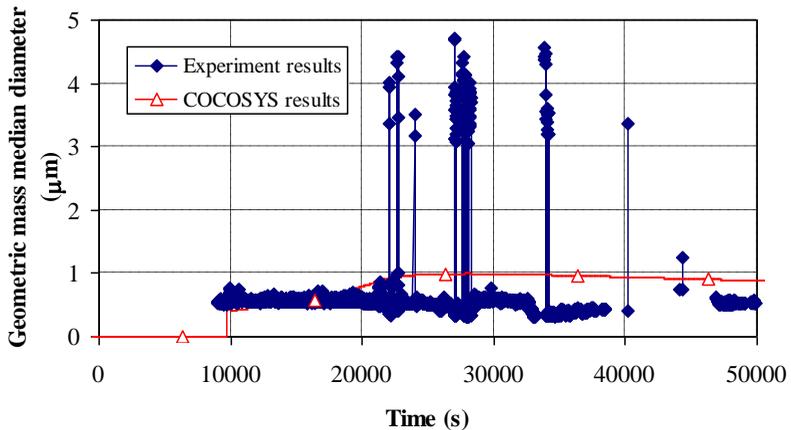
**Figure 6** Suspended aerosol mass in containment

In Figure 7 the distribution of airborne aerosol in the containment, obtained with ATLAS visualization tool, is presented in the time period of 11800 – 11950 s. The picture presents aerosol concentration and directions of the gas flows, which carry the particles. The aerosols to containment were injected through the pipe in R1H2 node below the condenser. The largest concentration of aerosol was observed above the pipe at the time of aerosol injection. Later the gas flows diffused in radial direction and the concentration of aerosol started to increase along. Some part of aerosol deposited down and some part was taken by the gas flow close to hot external walls of the facility to the upper plenum and then descended down close to “wet” condenser. After 11950 s the aerosol were homogeneously distributed in the whole volume except the gas space above the sump, where the concentration was less.



**Figure 7** Evolution of aerosol concentration distribution

Figure 8 presents the measured and calculated results of aerosol average geometric mass median diameter (GMMD) in containment atmosphere. According to experiment results, the structure of the aerosol particle is predominantly spherical, with sizes typically ranging from 0.5 to 1  $\mu\text{m}$ . The observations showed that these very fine particles might be agglomerated to form particles of size up to 20  $\mu\text{m}$  [17]. The rate of aerosol deposition by natural processes is in most circumstances very sensitive to aerosol particle sizes. For particles ranging from 0.5 to 1  $\mu\text{m}$  dominated process was gravitational deposition.



**Figure 8** Aerosol geometric mass median diameter

Distribution of aerosol's deposition on different surfaces in containment is shown in Table 1. The largest aerosol deposition was on the containment floor around the sump, where 74% of aerosol were deposited. On the condensers and in the sump were deposited 14% of aerosol mass, while on the vertical containment walls and removed by the sampling only 12% of aerosol. The results received with COCOSYS shows a good agreement between calculation and experimental results for the particles deposition on the condensers surfaces and in SUMP, but calculated deposition of aerosol on the containment walls and an amount of aerosol removed by the sampling were significantly lower (1% instead of measured 12%) than in experiment. The deposition on the containment floor was overestimated in comparison with the measured results. The deposition on the external vertical walls was determined by the Brownian diffusive deposition, which was weak excepting for very small particles. The diffusive deposition of aerosol was larger than gravitational only for particles smaller than 0.1  $\mu\text{m}$ .

**Table 1** Distribution of aerosol's deposition

	Floor of containment	Condenser surfaces and sump	Containment walls + samplings
Experiment results	74.0%	14.0%	12.0%
COCOSYS results	86.0%	13.28%	0.72%

### 3.3. Uncertainty and sensitivity analysis

The probabilistic uncertainty analysis was performed with the SUSA software [18], based on Wilks' formula. The tolerance limit and confidence level selected for this analysis was 0.95. According to Wilks' formula minimum the number of calculations for two-sided tolerance limits in this case is 93 and 100. The calculations were made to obtain reliable uncertainty and sensitivity measures. Spearman's rank correlation coefficients are presented as a measure of sensitivity. Spearman's rank correlation coefficient is an ordinary product moment correlation coefficient computed on rank transformed data. Spearman's coefficient shows how well two variables are monotonically related [19].

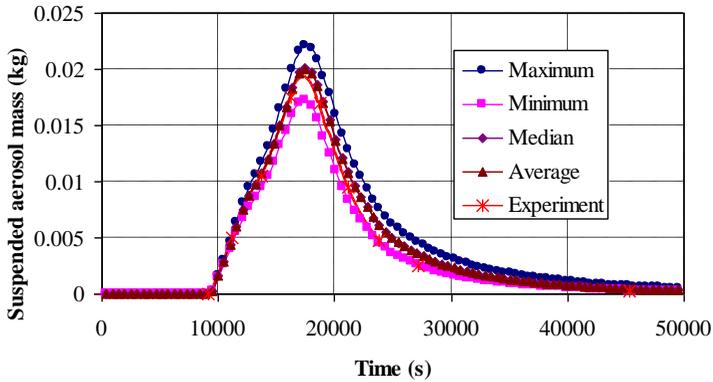
Table 2 presents the list of 24 parameters with expected values and probabilistic range of values. All parameters were investigated with the Normal (Gaussian) probabilistic distribution.

**Table 2** Parameters of uncertainty and sensitivity analysis

Nr.	Parameter	Expected value	Min. value	Max. value
1	Solubility factor of soluble aerosol	1.73	1.45	2.0
2	Dynamic shape factor	1.0	0.84	1.16
3	Particle sticking probability factor	1.0	0.84	1.16
4	Particle agglomeration factor	1.0	0.84	1.16
5	Average aerosol density, kg/m <sup>3</sup>	3000	2520	3480
6	Mass median diameter, m	$2.02 \cdot 10^{-6}$	$1.69 \cdot 10^{-6}$	$2.34 \cdot 10^{-6}$
7	Geometric standard deviation	2.0	1.68	2.32
8	Aerosol size classes	20	17.0	20
9	Molecular weight of soluble components, g/mol	118	99.12	136.8
10	Molecular weight of non-soluble components, g/mol	114	95.76	132.24
11	Diffusive boundary layer thickness, m	$1.0 \cdot 10^{-4}$	$1.0 \cdot 10^{-5}$	$1.0 \cdot 10^{-3}$

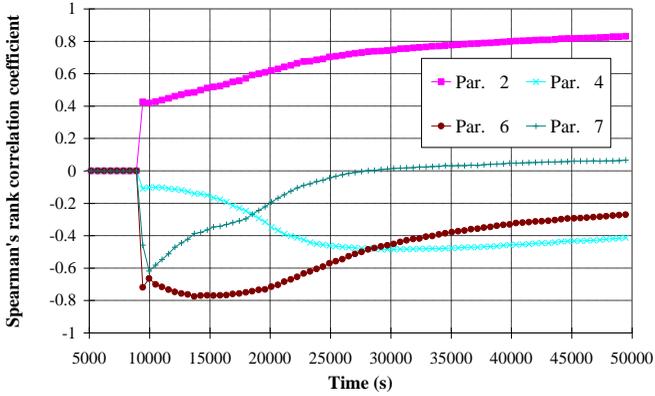
12	Particle slip coefficient	1.37	1.15	1.58
13	Average thickness of water films, m	$3.0 \cdot 10^{-4}$	$2.52 \cdot 10^{-4}$	$3.48 \cdot 10^{-4}$
14	Molecular weight of gas, g/mol	20.35	17.0	23.0
15	Turbulence dissipation rate, $m^2/s^3$	0.02	0.0168	0.0232
16	Initial average temperature, °C	108.0	107.0	109.0
17	Humidity, %	51.29	50.29	52.29
18	Initial average pressure, bar	1.95	1.85	2.05
19	Total loss coefficient per atmospheric junction	1.5	1	2
20	Water quantity in sump, ltr	120.0	110.0	130.0
21	Inner walls temperature in sump, °C	90.0	89.0	91.0
22	Containment walls temperature, °C	110.0	109.0	111.0
23	Condensers („wet“ part) temperature, °C	90.0	89.0	91.0
24	Condensers („dry“ part) temperature, °C	120.0	119.0	121.0

Figure 9 reveals the results of uncertainty analysis: calculated suspended aerosol mass maximum, minimum, average, median values and measured values in experiment. Initially, calculated aerosol mass median values agreed with measured values, but after 17600 s calculated aerosol mass median values were lower than the measured values. At the end of calculation minimum aerosol mass median values agree with the minimum experimental values. Maximum calculated suspended aerosol mass after ~17600 s was ~0.022 kg, the calculated minimum suspended aerosol mass was ~0.017 kg and the maximum measured mass was ~0.019 kg.



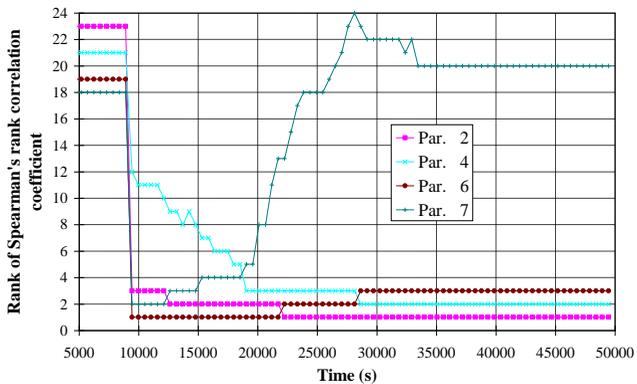
**Figure 9** Suspended aerosol mass (maximum, minimum, median, average and experiment values) in containment

The results of sensitivity analysis of suspended aerosol mass are presented in Figure 10 and Figure 11. In Figure 10 are presented 4 parameters, which have the largest influence (Spearman's coefficient is larger than  $\pm 0.3$  at least in one point) on suspended aerosol mass. These parameters are: dynamic shape factor (parameter No. 2), particle agglomeration factor (parameter No. 4), mass median diameter (parameter No. 6) and geometric standard deviation (parameter No. 7). Received results confirm with results from VANAM experiments [20]. After 9000 s the Spearman's rank coefficient of dynamic shape factor increases from 0.4 to  $\sim 0.8$ . The average particle density has the largest impact in the time range from 10000 till 25000 s, when a coefficient varies from -0.8 to -0.6. After 22000 s Spearman's rank coefficient of particle agglomeration factor varies in range from -0.5 to -0.4. The geometric standard deviation effect is largest only in the beginning of calculations, to 1400 s.



**Figure 10** Spearman's rank correlation coefficients for suspended aerosol mass (only the parameters with coefficient exceeding 0.3 at least at one point are highlighted)

Rank of Spearman's rank correlation coefficients for suspended aerosol mass of 4 most important parameters is presented in Figure 11. Initially, till 22000 s, the largest influence is in the mass median diameter (parameter No. 6). After 22000 s the strongest influence on the suspended aerosol mass has dynamic shape factor (parameter No. 2) and particle agglomeration factor (parameter No. 4), because the form and size of particles have strongly changed in comparison to the initial parameters. Geometric standard deviation (parameter No. 7) has larger influence only in the first phase of calculation, when the influence of initial particle parameters is still intense.



**Figure 11** Rank of Spearman's rank correlation coefficients for suspended aerosol mass

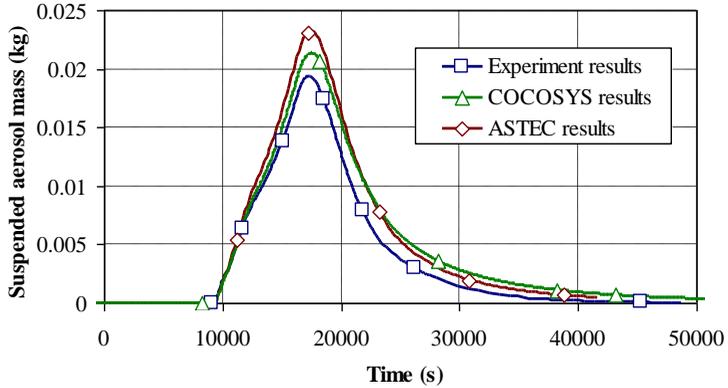
The distribution of aerosol deposition on different surfaces in containment is shown in Table 3. The largest deposition of aerosol was on the containment floor around the sump, where 74% of aerosols were deposited. There were deposited 14% of aerosol mass on the condensers and in the sump, while on the vertical containment walls and removed by the sampling were only 12% of aerosol mass. The results received with SUSA program showed the range of minimum till maximum values of aerosol deposition on different surfaces. The deposition of particles on the containment bottom varied in range from 71.44% till 86.88% and depended mainly on factors of sticking probability, dynamic and geometric shape. The deposition on the condenser surfaces and sump varied in range from 11.28% till 16.28%. The estimated deposition on the containment walls varied from 0.42% till 0.9%. The range of deposition on the condenser surfaces mainly depended on previously mentioned factors plus a slip factor. The deposition of particles on the containment walls was conversely proportional to particle diameter and directly to diffusion boundary layer, but the observed deposition was less than the one measured in the experiment.

**Table 3** Distribution of aerosol’s deposition

	Floor of containment	Condenser surfaces and sump	Containment walls + samplings
Experiment	74.0%	14.0%	12.0%
Min	71.44%	11.28%	0.42%
Max	86.88%	16.28%	0.9%

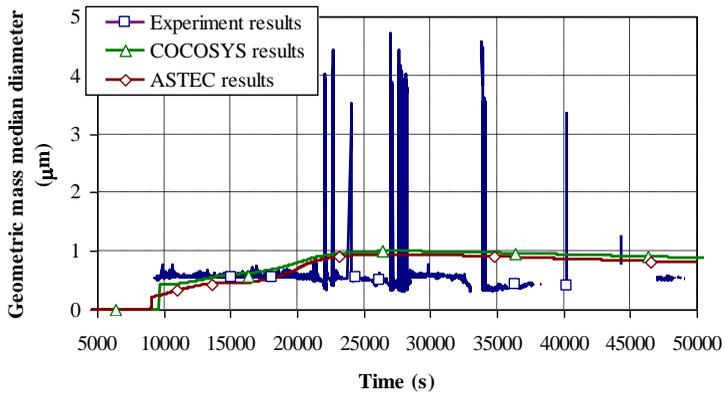
### 3.4. Comparison of aerosol transport calculation using COCOSYS and ASTEC codes

In Figure 12 the comparison of suspended aerosol mass calculation using COCOSYS and ASTEC codes with measured results is presented. Maximum observed value of the airborne aerosol mass in containment was after ~17600 s. The measured airborne aerosol mass was below calculated results during all analyzed period, but the difference was less than 5 g. The maximal measured mass was ~19 g, while calculated using COCOSYS code was ~21 g and by using ASTEC code was ~23 g. After ~22000 s from the beginning of the test, aerosol mass measured by using ASTEC code was less than aerosol mass calculated by COCOSYS and it shows, that deposition rate was faster with ASTEC code, but, anyway, both calculated results were similar to the results of the experiment.



**Figure 12** Aerosol mass suspended in the containment atmosphere

Figure 13 presents the measured and calculated results of aerosol average geometric mass median diameter (GMMD) in containment atmosphere. According to the measured results the structure of the aerosol particle was predominantly ball shaped, with sizes typically ranging from 0.5 to 1  $\mu\text{m}$ . The calculated result was ranging from 0.5 to 1  $\mu\text{m}$  because of agglomeration processes. Difference between calculated results, using COCOSYS and using ASTEC codes, were only minor.



**Figure 13** Aerosols geometric mass median diameter in containment atmosphere

Distribution of aerosol deposition on different surfaces in containment is shown in Table 4. The largest aerosol deposition was on the containment floor around the sump, where 74% of aerosols were deposited. 14% of aerosol mass

were deposited on the condensers and in the sump, while on the vertical containment walls and removed by the sampling were only 12% of aerosol mass. The results received with COCOSYS shows a good agreement between calculation and experimental results for the particles deposition on the condensers surfaces and SUMP, but deposition on the containment walls and the deposition of aerosol mass, removed by the sampling, were significantly lower (0.72% instead of measured 12%), while deposition on the containment bottom was overestimated. The results received with ASTEC code showed parallel results. Nevertheless, the deposition on the containment bottom was ~3% lower and was similar to the results of the experiment. The deposition on the condensers and SUMP received with ASTEC code was overestimated comparing with COCOSYS result, but the difference was less than 1%. The diffusive aerosol deposition on the vertical containment walls was also underestimated. The aerosol deposition results with ASTEC code transcend the COCOSYS results more than twice. The model, implemented in ASTEC code, gives better possibility to precisely evaluate deposition distribution and could be implemented in other computer codes.

**Table 4** Distribution of aerosol deposition

	Floor of containment	Condenser surfaces and sump	Containment walls + samplings
Experiment	74.0%	14.0%	12.0%
COCOSYS	86.0%	13.28%	0.72%
ASTEC	82.98	14.88	2.14

#### 4. CONCLUSIONS

In order to investigate the processes of aerosol and radionuclides transport in the containments of the nuclear power plants the numerical study has been carried out. There experimental results of PHEBUS FPT-1 and FPT-2 were used for this numerical analysis. The obtained numerical results were compared with experimental values and formulated the following conclusions:

1. In containment numerical model design is necessary to evaluate convectional gas flows, which directly influence deposition processes of aerosol and radionuclides.
2. The carried out investigation of PHEBUS FPT-1 and FPT-2 experiments revealed that the density of aerosols, the coefficient of solubility and the thickness of diffusion's layer have only insignificant impact on the deposition of aerosols and radionuclide.
3. The performed uncertainty analysis revealed that with possibility of 95% deposition on the floor of the containment was within the range

from 71% to 86%, when deposition on the floor during the experiment was 74%; calculated deposition on the surface of the condenser and of the sump was within the range from 11% – 16%, when in the experiment it was 14%; calculated deposition on the walls was within the range from 0,4% – 0,9%, when in the experiment it was 12%.

4. The carried out sensitivity analysis highlighted the parameters, which have the biggest impact on:
  - Suspended aerosol mass variation – dynamic shape factor, particle agglomeration factor, mass median diameter and geometric standard deviation;
  - Aerosol deposition on the containment floor – dynamic shape factor, particle agglomeration factor, mass median diameter and geometric standard deviation;
  - Aerosol deposition on the condenser surfaces and sump – dynamic shape factor, particle agglomeration factor, average thickness of water films and initial average pressure;
  - Aerosol deposition on containment walls – geometric standard deviation and diffusive boundary layer thickness.
5. The model of diffusive deposition, installed in ASTEC code, enables to evaluate the heterogeneous structure of the boundary layer, where aerosol and radionuclides are gradually suppressed, and consequently the deposition of particles on vertical walls (>2%, the FPT-2) in comparison with model, installed in COCOSYS program, (<1%, the FPT-2), therefore it is recommended to install a new model of diffuse deposition in the COCOSYS program package.
6. Recommendations for numerical model design:
  - If the inlet flow of aerosol and radionuclides is located in the central part of compartment, then in numerical model it is recommended to define three or more radial subdivisions.
  - Detailed “free jet” model in aerosol and radionuclides transport simulation is not recommended, because it causes too small nodes and leads to systemic errors.
  - If humidity in the analyzed compartments is less than 85% and hygroscopic components make up less than 5%, then all aerosols could be modeled as single aerosol component and the steam condensation on aerosols could be neglected.

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2002 – 2006 studied at Kaunas University of Technology, Faculty of Fundamental Sciences, Department of Physics, and was granted Bachelor's degree.

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## Reziumė

Atominių elektrinių (AE) eksploatacija yra susijusi su rizika, kad įvykus avarijai su šilumnešio praradimu, radioaktyvios medžiagos pasklis už atominės elektrinės ribų. Siekiant apsaugoti nuo radioaktyvių medžiagų patekimo už jėgainės ribų būtina suprasti branduolinėse jėgainėse avarijų metu vykstančius reiškinius.

Didžiausia tikimybė radioaktyvioms medžiagoms pasklisti už jėgainės ribų yra būti pernešamoms kartu su aerozolių srautu. Aerozoliai yra mažos kietos arba skystos dalelės sklendinčios dujose, kurių dydis dažniausiai apibrėžiamas srityje nuo 0,01 μm iki 100 μm. Atominėse elektrinėse paskutinis barjeras, neleidžiantis šių medžiagų pasklidimui už jėgainės ribų, yra apsauginis kiautas. Apsauginis kiautas yra cilindrinis gelžbetoninis statinys, gaubiantis reaktoriaus aušinimo kontūro vamzdyną ir patį reaktorių. Trūkus reaktoriaus aušinimo kontūro vamzdynui, radioaktyviomis medžiagomis užterštas šilumnešis išteka į apsauginį kiautą, kuriame radioaktyvios medžiagas turi būti išlaikomos tol, kol jos bus nukreiptos į valymo įrenginius arba jų aktyvumas nesumažės dėl natūralių radioaktyvaus irimo procesų.

Aerozolių ir radionuklidų pasiskirstymas branduolinių jėgainių apsauginiuose kiautuose yra tiriamas jau daugelį metų. Šių procesų tyrimams yra vykdomos įvairios eksperimentinės ir skaitinės tyrimų programos (DEMONA, KAEVER, OECD-THAI, PHEBUS). Skaitiniams tyrimams apsauginiuose kiautuose atlikti dažniausiai yra taikomi suvidurkintų parametrų programų paketai (COCOSYS, ASTEC, MELCOR, CONTAIN ir kiti), kurie per pastaruosius 20 metų stipriai patobulėjo, tačiau vis dar nėra sukurta bendra metodologija, vieningai pagrindžianti šių programų paketų naudojimą aerozolių ir radionuklidų pernašos reiškiniams apsauginiame kiaute tirti.

Šiame darbe yra atliktas skaitinis aerozolių ir radionuklidų pernašos procesų tyrimas pasinaudojant PHEBUS eksperimentiniame stende atliktais FPT-1 ir FPT-2 eksperimentų rezultatais. Atlikta parametrinė dalelių nusėdimo greičio ir pasiskirstymo analizė. Pateikti siūlymai naudoto COCOSYS programų paketo tobulinimui ir skaitinio modelio, naudojamo aerozolių ir radionuklidų pernašos procesų modeliavimui, sudarymui.

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