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Content

1 INTRODUCTION

Today, about 80% of all energy produced comes from the fossil fuel (oil, carbon, and natural gas). European scientists are developing environmentally friendly, safe, and renewable energy technologies. Nuclear fusion is one of them. Nuclear fusion reactors promise high power energy sources, which have low impact on environment, are safe and have virtually unlimited fuel resources. This technology is not limited to heat and electricity generation, it also could be used for hydrogen production, which would lead to further development of the "hydrogen economy".

European nuclear fusion research program allows using common European research and their development resources in all important research areas. Co-operation is especially important not only in the operation of the Joint European Torus (JET), but also in the execution of the European Fusion Development Agreement (EFDA) technological program, which is devoted to the ITER project, and also encompasses promising DEMO research. European fusion research and development program, based on EURATOM contract, is being coordinated and carried out by the European Commission.

After negotiations took place in the year 2006, Lithuanian Energy Institute (LEI) signed a contract on joining the EFDA agreement. On 2006 November 15, the first meeting of this project with the participation of the European Commission and Lithuanian organizations took place. During this meeting, project execution rules were presented and work programs for the year 2007 were agreed. The signed contract came into force from 1st January 2007 and Lithuania has officially become an EFDA member.

Following signed contract, work program is composed every year and approved by the supervision committee.

Currently, there are two Lithuanian organizations participating in the EFDA project – Lithuanian Energy Institute and Vilnius University Institute of Theoretical Physics and Astronomy. Information regarding works performed by both these institutions during the year 2008 is presented in this report.

2 ACCIDENT ANALYSIS AND EVALUATION OF CONSEQUENCES FOR W7-X

2.1 Analysis of 40 mm pipe rupture during "baking" mode operation

W7-X (Figure 2.1) is a stellarator type nuclear fusion experimental device, currently being built at the Max Planck Institute of Plasma Physics (Max-Planck-Institut für Plasmaphysik (IPP), in Greifswald, Germany. The purpose of this facility is to demonstrate that stellarator type devices can be used to sustain stable plasma conditions for half an hour and longer. Plasma diagnostics and control technologies would be tested in this facility. Protective plates and cooled components of first wall used inside the plasma torus are made from the same materials, which will be used for the ITER facility; therefore, W7-X will also contribute to the ITER development.

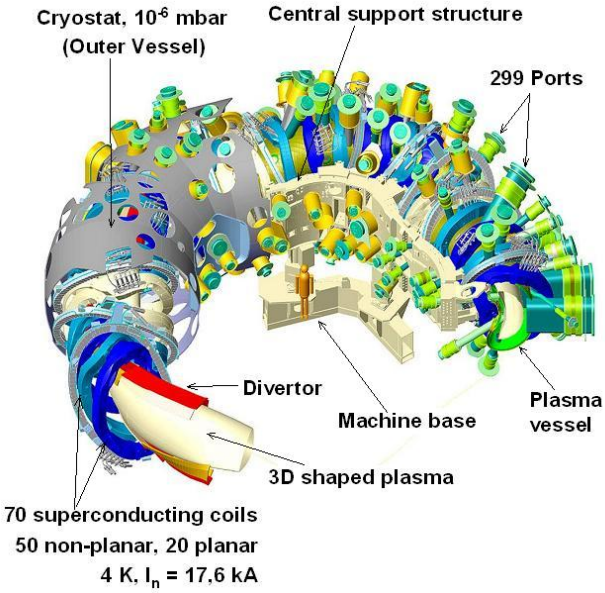


Figure 2.1 The fragment of a CAD model of the W7-X system

Co-operation between LEI and IPP started in the year 2007 and were continued during the year 2008. It was planned to perform an analysis of the cooling water pipe rupture with the aim of estimating the amount of the coolant flowing into the torus and evaluating if the area of the planned burst disk is sufficient in order to prevent torus overpressure. IPP gave all required information for the calculations about the piping of the W7-X facility. If needed drawings were not yet developed, instead modelling assumptions were made.

It is considered in the project that a rupture of one 40 mm diameter pipe, providing water to the divertor target is the most severe accident in terms of vacuum vessel pressurization [1]. In order to avoid negative effects on device equipment absolute pressure inside the torus must not exceed 1.1 bar. To avoid the plasma vessel overpressure, active (safety valves on coolant pipes) and

passive safety devices (burst or rupture disk) are used. The burst disk has to be opened at 1.1 bar pressure inside the torus and relief steam into the torus hall, i.e. room in which W7-X is situated. Steam can be released from the torus hall with the means of ventilation or through the safety valves.

During one of the LEI and IPP meetings it was decided that LEI will perform analysis of the 40 mm diameter pipe rupture during the W7-X operation mode "baking" and will also perform strength analysis of the 12 mm diameter pipe [2]. "Baking" mode of the device operation is used in order to preheat constructions of the torus and to clear the volume of the plasma before its initialization. RELAP5 [3] and COCOSYS [4] program codes were used for the pipe rupture analysis. RELAP5 was used to obtain coolant flows in the coolant system piping and parameters of the coolant flowing through the rupture (mass flow rate and specific enthalpy). Information obtained from the RELAP5 code calculation was used further performing calculations with the COCOSYS program code, which is suitable to obtain evolutions of the thermodynamic parameters inside the plasma vessel and torus hall.

In Figure 2.2 there is shown a layout of the W7-X device cooling circuit and "baking" circuit. This scheme and other project information was analyzed and discussed with the IPP specialists. Information was later systematized and model of the piping system was developed for the RELAP5 computer code. The general scheme of the W7-X device cooling and "baking" circuits are shown in Figure 2.3. It was used performing the analysis of the 40 mm diameter pipe rupture. With the aim to analyse rupture of the pipe, one of the five modules was modelled in more details (Figure 2.4). In this module, target elements were separated and an assumption that the ruptured pipe was providing coolant for the upper 1TH element (model element "136") was made. The rupture was simulated by making assumption that during the accident the valve "198" is opened and coolant flows into the volume, which is indicated as "199" in the model. Parameters of the cooling circuit during the "baking" regime were given in the project documentation as follows: pressure in the piping 10 bar, coolant temperature 160 ^{0}C, coolant flow in the piping – 1382 m^3/hour (348 kg/s). Water flow in the "baking" circuit – 177 m^3/hour (44.6 kg/s).

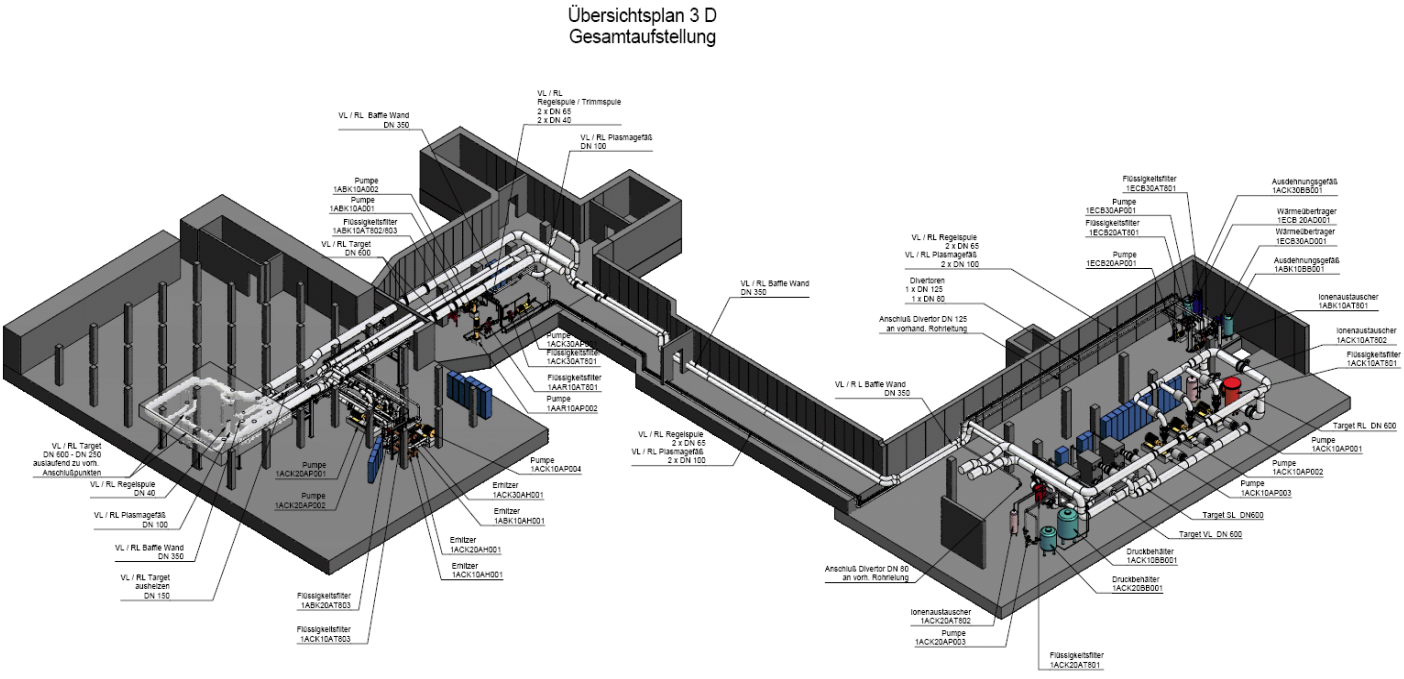


Figure 2.2
Layout of the W7-X device cooling circuit and "baking" circuit

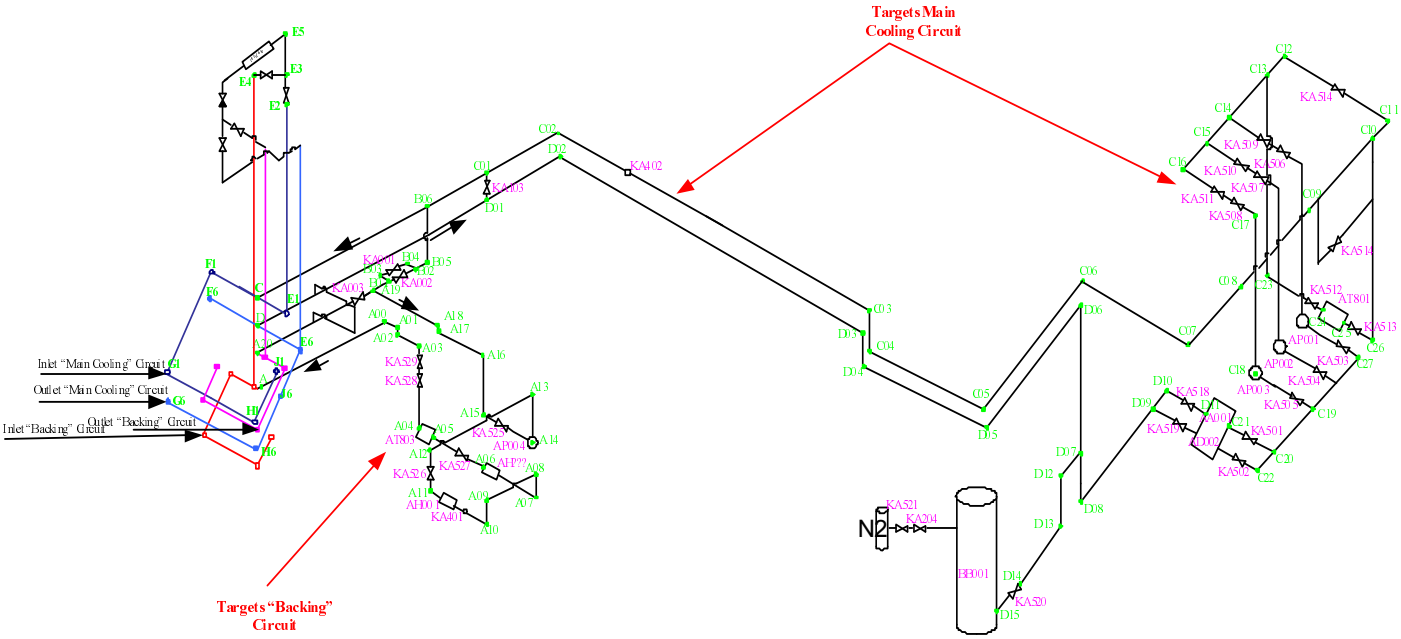


Figure 2.3
RELAP5 nodalisation scheme of the cooling and "baking" circuits

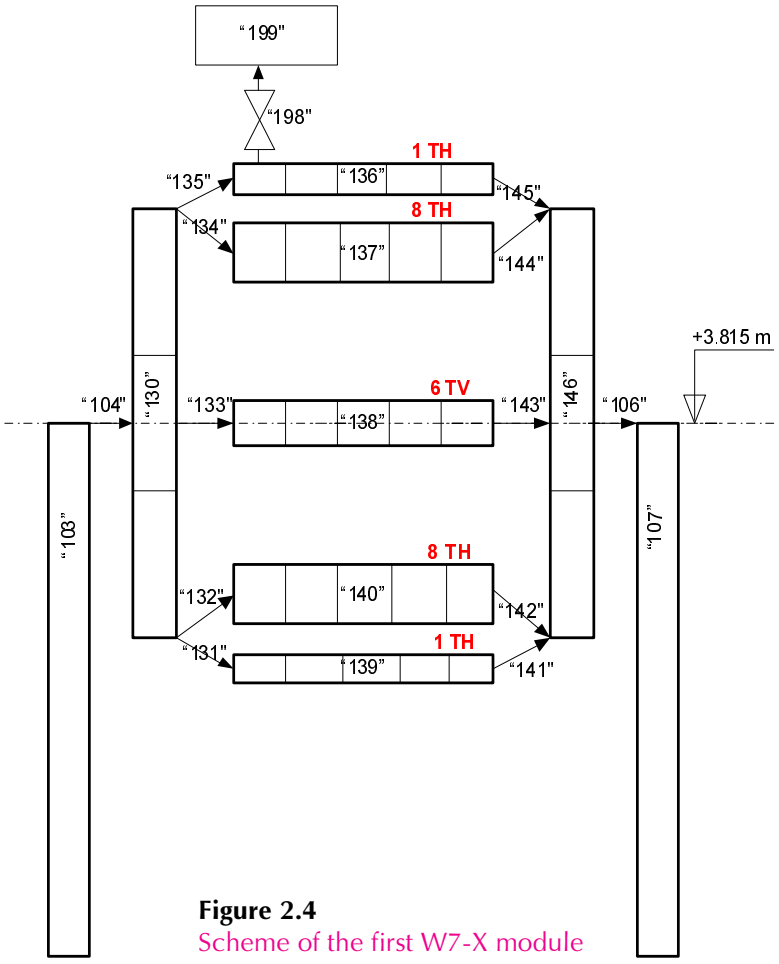


Figure 2.4
Scheme of the first W7-X module

Performing the analysis of the accident an assumption was made that the pipe rupture takes place at the start of the calculations (0 s), and after 2 s, due to pressure increase inside the torus, emergency alarm is raised and safety valves are closed in the piping. 3 s after the signal raising valves are fully closed. 10 s after the accident started "baking" circuit pumped is stopped.

Figure 2.5 – Figure 2.7 presents main results obtained from the RELAP5 calculations. Figure 2.5 shows steam volume fraction evolution inside the ruptured pipe. Until the pipe becomes ruptured, water is flowing inside the pipe. After the rupture, pressure inside the pipe decreases and causes water to partly evaporate, and after 60 s only steam is flowing out of the rupture.

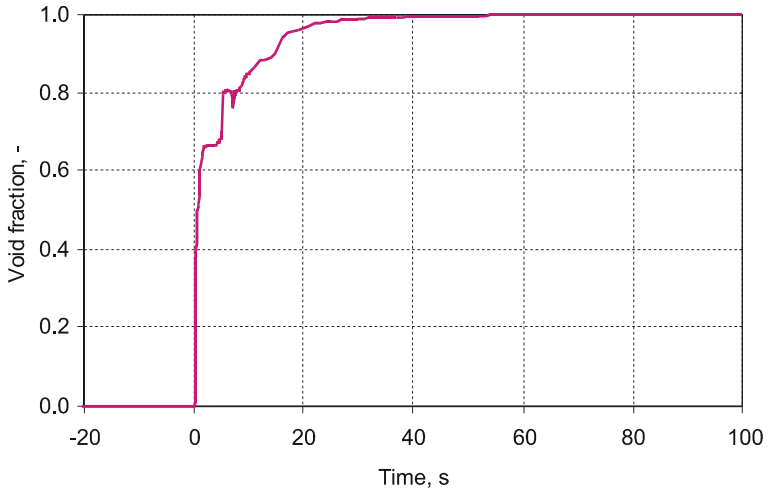


Figure 2.5
Steam volume fraction of the coolant, flowing through the pipe rupture

Figure 2.6 presents evolutions of the coolant steam volume fractions in the different targets of the affected module. First, water flows out from the upper parts of unaffected targets (curve "8TH top") and only later from the affected target (curve "1TH top"). This happens because those targets are interconnected and coolant from the unaffected targets flows out through the affected target. Later on, coolant also flows out from the vertical side targets (curve "6TV"), however part of the water stays in lower targets.

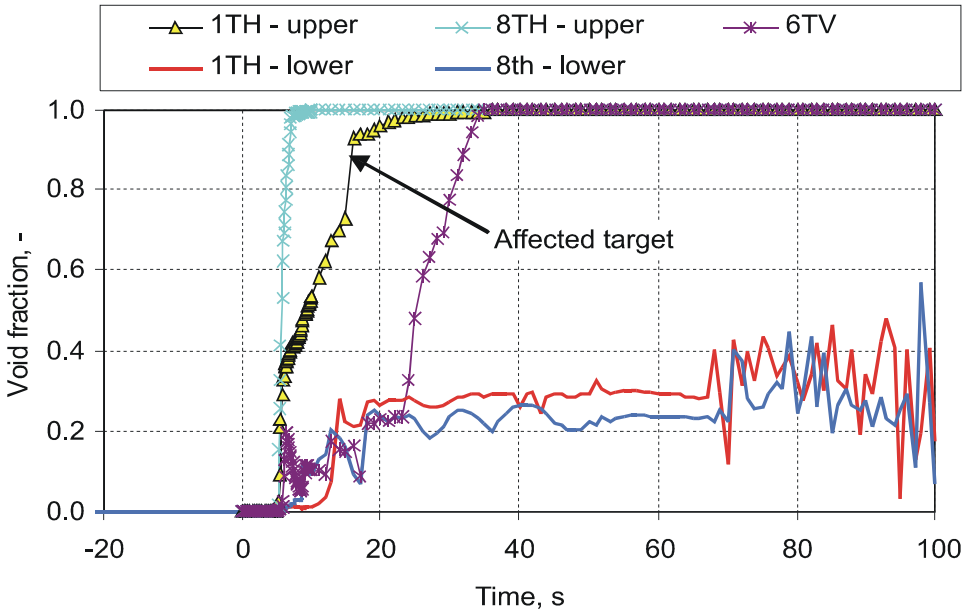


Figure 2.6
Steam volume fraction of the coolant in the different targets

Figure 2.7 shows results of the RELAP5 calculations, presenting parameters of the coolant flowing through the pipe rupture – mass flow rate and specific enthalpy. These parameters were necessary in order to perform further calculations of the evolution of thermodynamic parameters inside the torus and torus hall.

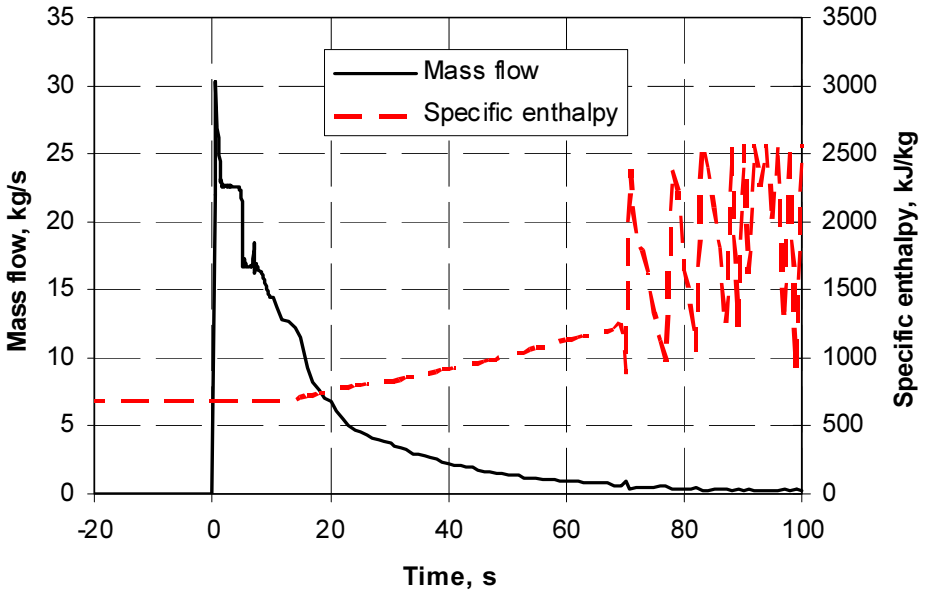


Figure 2.7
Mass flow rate and specific enthalpy of the coolant flowing through the pipe rupture

Figure 2.8 presents torus volume model for the COCOSYS code. This model has been developed with an assumption that vacuum vessel has a cylindrical shape, i.e. complicated three-dimensional geometry of the stellarator is neglected. However, whole volume, surface area, and mass of the structures have been used in the model according to the available project data. Figure 2.8 shows the cross-section view of only one module, however all five modules have been included into the model. Modeling assumption has been made that after the rupture coolant flows out into the first module, control volume OTR, i.e. the right side of the upper part.

Since during the "baking" mode of the device pressure in the cooling circuit is 10 bar, but inside the torus it is 10^{-4} mbar, coolant flowing out through the rupture partly evaporates. The part coolant, which does not evaporate, impacts the hot steel structures and partly evaporates. Steam generated due to this coolant evaporation increases pressure inside the vacuum vessel.

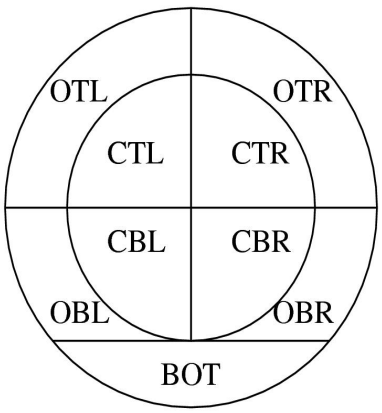


Figure 2.8
Cross-section view of the torus model for the COCOSYS code

Assumption has been made that initial pressure inside the pressure vessel is 1000 Pa, i.e. lower than atmospheric pressure, initial temperature of gas and structures – 150 ^{0}C. Burst disk is placed in the wall of the third module control node OTL, i.e. the left side of the upper part of the module. Valve is opened when the absolute pressure inside this node reaches 1.1 bar.

Calculation results, presented in Figure 2.9 – Figure 2.11, were obtained from the calculations performed with the COCOSYS code. Figure 2.9 shows evolution of the pressure inside the torus after the rupture of the 40 mm diameter pipe. After the pipe has ruptured, pressure inside the vacuum

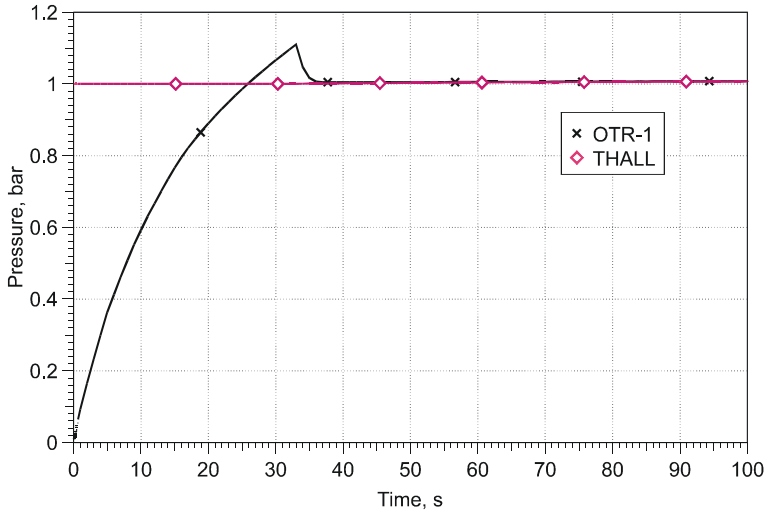


Figure 2.9
Pressure inside the torus volume (OTR-1) and torus hall (THALL)

vessel starts to increase and after 25 s reaches atmospheric value (curve "OTR-1"). After the 33 s pressure reaches 1.1 bar and burst disk is opened. After the activation of the burst disk, pressure inside the torus decreases to atmospheric. These results show that planned burst disk is sufficient in order to avoid the increase of pressure in excess of 1.1 bar. After the burst disk activation pressure inside the torus hall (curve „THALL") starts to increase, however this increase is not significant, because the volume of the torus hall is very large, ~16800 m^3.

Figure 2.10 illustrates evolution of the steam mass flow through the burst disk. It opens 33 seconds after the pipe rupture. Maximum mass flow rate through the disk reaches ~3.7 kg/s and after that is constantly decreasing till the end of calculation. Small oscillations of the mass flow rate starting to occur 70 seconds after the rupture are caused by the fluctuations of the specific enthalpy of the coolant flowing out of the rupture (Figure 2.7).

Figure 2.11 presents the evolution of the water mass in the lower part of the W7-X torus first module. During the first 20 seconds, there is small amount of water in the lower part of the first module. The reason for this is that part of the water flowing out of the rupture evaporates due to the lower pressure and the interaction with the hot structures. It is considered in the developed COCOSYS model that water can flow from the higher structures to the lower ones Taking into account these factors, one can obtain that water in the lower part of the first module begins to

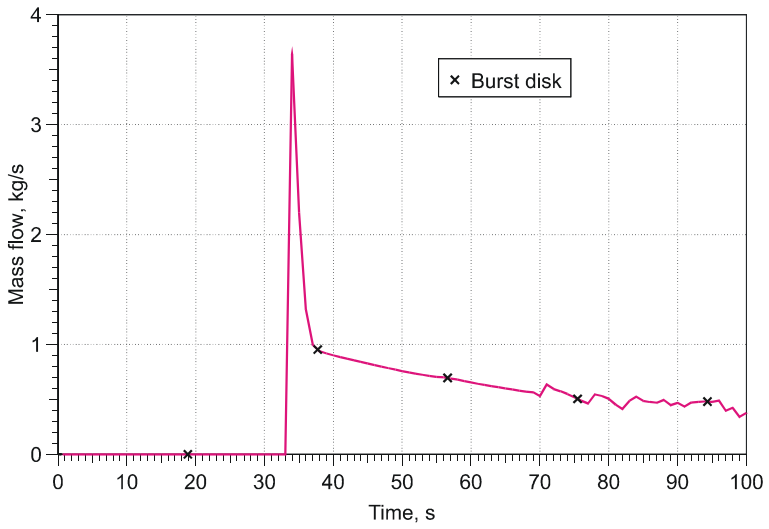


Figure 2.10
Steam mass flow rate, flowing out through the burst safety disk

collect only 20 s after the rupture have taken place. 100 s into the accident there are ~63 kg of water collected in the lower part of the first module.

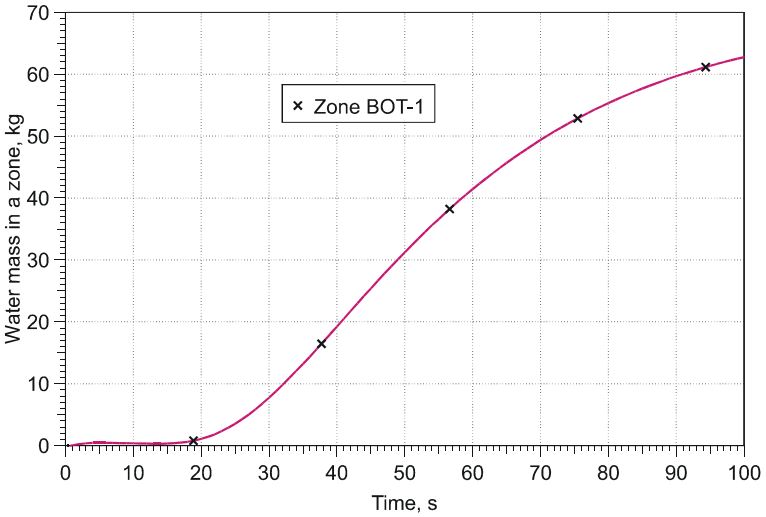


Figure 2.11
Evolution of the water mass in lower part of the torus

2.2 Leak before break analysis

The upper part of the target module 1H (see **Figure 2.12**) was selected for the leak before break (LBB) analysis. The geometrical modelling was performed using SolidWorks computer program [5]. The geometrical model of upper part of target pipeline depicted in **Figure 2.13**. The upper part of 1H module pipeline consist of seven small 10 mm diameter pipes connected to 40 mm diameter collector.

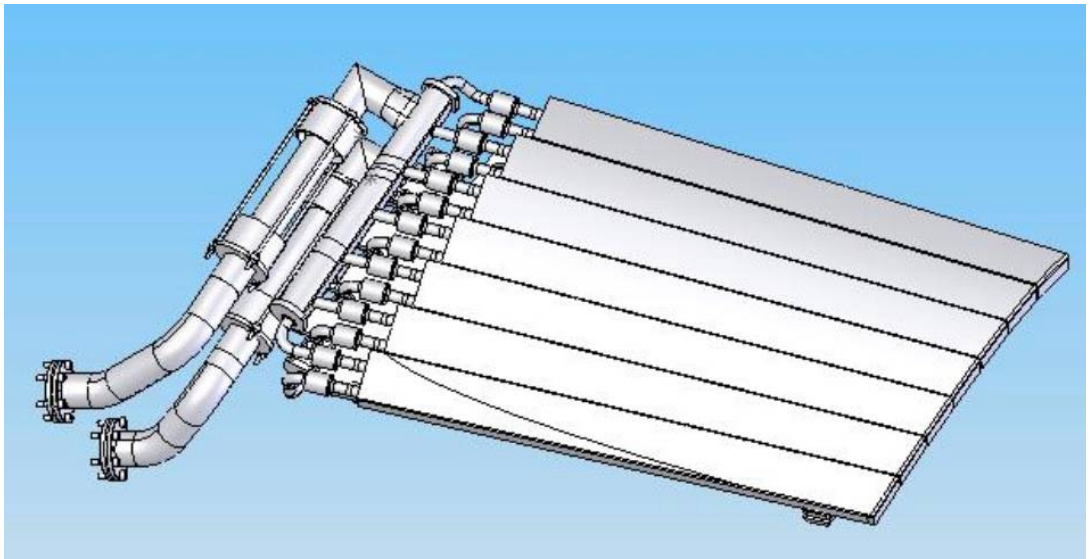


Figure 2.12 General view of the target module 1H

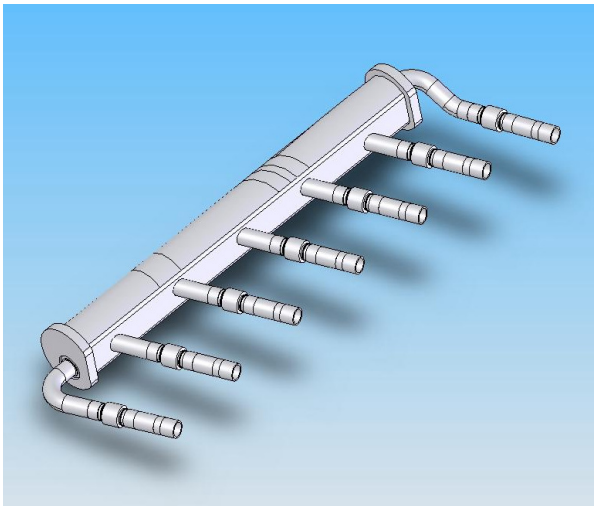


Figure 2.13
Model of target module 1H upper pipeline

The mechanical properties of stainless steel 316L were used for the FE analysis. The mechanical properties of this steel are summarized in Table 2.1.

Table 2.1. Material Properties of steel 316L

Modulus of elasticity, GPa	Yield strength, MPa	Tensile strength, MPa	Poisson's ratio
205	147	500	0.3

The pressure inside the pipeline of 28 bar and the vacuum environment of 10^{-7} bar are the main loads in the real construction. To evaluate these both loads the static pressure of 2.9 MPa was applied inside the pipeline in the FE model. The temperature of 160° C was also considered.

Stress analysis of the target module 1H in case operational loading was performed using a finite element method (software COSMOSWorks). The results of van Misses stresses distribution of target module is shown in Figure 2.14. The biggest stresses were received in the pipes of 10 mm diameter. Enlarged view of most loaded part is shown in Figure 2.15. As we can see in this figure,

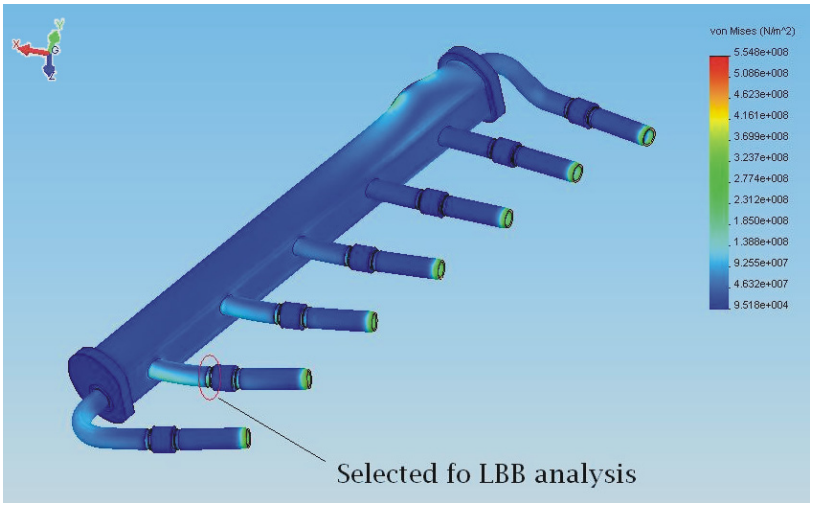


Figure 2.14
Distribution of von Misses stresses in the 1H module upper pipeline

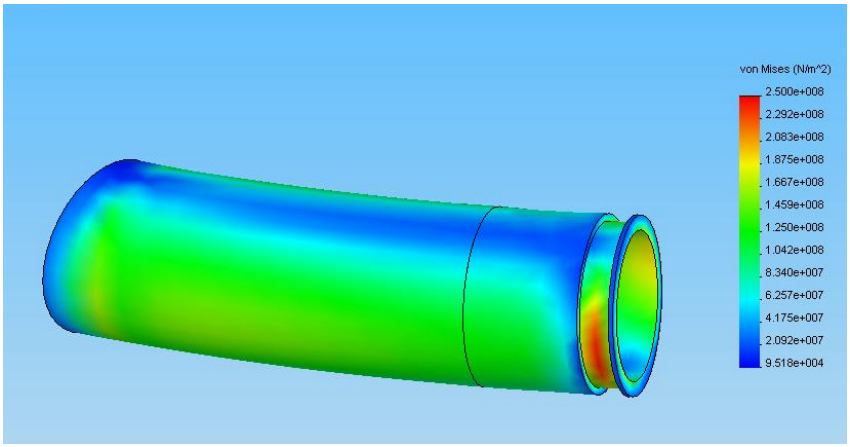


Figure 2.15
Distribution of von Misses stresses in the most loaded pipeline

the maximum value of stresses is in connection of the pipe with expansion joint and reach 250 MPa. The high value of the stresses was received because of conservative assumption of boundary condition and small thickness of joining pipe. The objective of this analysis was selection of most loaded zone only, therefore the results of analysis can be used and more detailed analysis is not needed. The marked zone was selected for LBB analysis.

The analysis of the critical and acceptable crack sizes was based on engineering safety assessment procedure R6 [6, 7]. The fallowing data was used in this analysis:

- Geometrical shape: cylindrical pipe with inner diameter of 10 mm and wall thickness of 1 mm;
- Material properties: stainless steel 316L;

Fracture parameters: due to insufficient data the stress intensity factor of 97 MPa·m$^{-1/2}$ was assumed as austenitic stainless steel pipes of Ignalina NPP. The through-wall crack was analysed at loads of normal operation, i.e. the pressure inside the pipeline of 28 bar and the vacuum environment of 10^{-7} bar. During this analysis the acceptable through-wall crack length of 1.4 mm and critical of 6.5 mm were obtained. The results of this analysis are shown in Figure 2.16.

The deterministic LBB analysis was performed according to recommendations [8, 9, 10] for application of the Leak Before Break concept. The basic aim of LBB analysis is that flow through

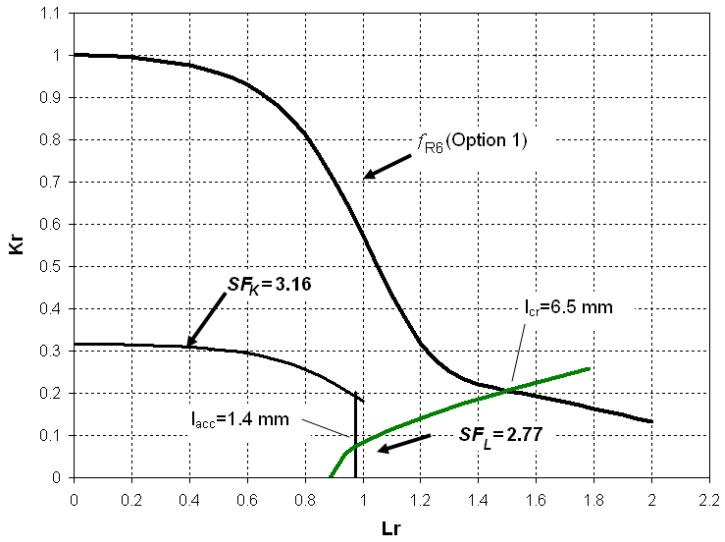


Figure 2.16
Distribution of von Misses stresses in the most loaded pipeline

through-wall crack must be detected before crack will reach the critical sizes. Analysis is performed for the postulated through-wall cracks.

The function of crack opening is one of the basic initial data for leak rate calculations. To obtain this function elastic-plastic finite element analysis was performed for the most loaded part of analysed construction. The CASTEM 2000 code was used for this analysis [11]. The analysis was performed at loads of normal operation, i.e. the pressure inside the pipeline of 28 bar and the vacuum environment of 10^{-7} bar. The analysis results are presented as stress snapshots. The von Misses stresses in the pipe with through crack are presented in Figure 2.17. The maximum stresses were received at tip of the crack and reached 140 MPa.

The function of crack opening is constructed for target module 1H pipe using normal operation loading. The results of analysis are presented in Figure 2.18.

The leak rate through the crack is determined for normal operation conditions. For leak rate calculations the computer program SQUIRT v.2.4 was used [12]. It was considered that the crack opening is of elliptical shape, the wall thickness is equal to 1 mm, and discharge coefficient is equal to 0.95. The calculations were performed using crack opening function as shown in Figure 2.18. Calculated leak rates are presented in Figure 2.19. According to this function the leak rate through acceptable crack is 0.1 kg/h and through critical crack is 1.4 kg/ h.

According to LBB requirements the postulated through-wall crack length, at which necessary leak rate is reached, should be less than half-length of critical through-wall crack. The leak rate through acceptable crack is 0.1 kg/h. The vacuum environment is inside of the plasma vessel and this leakage inside of the plasma vessel will be detected immediately. The acceptable through-wall crack length (1.4 mm) is more than

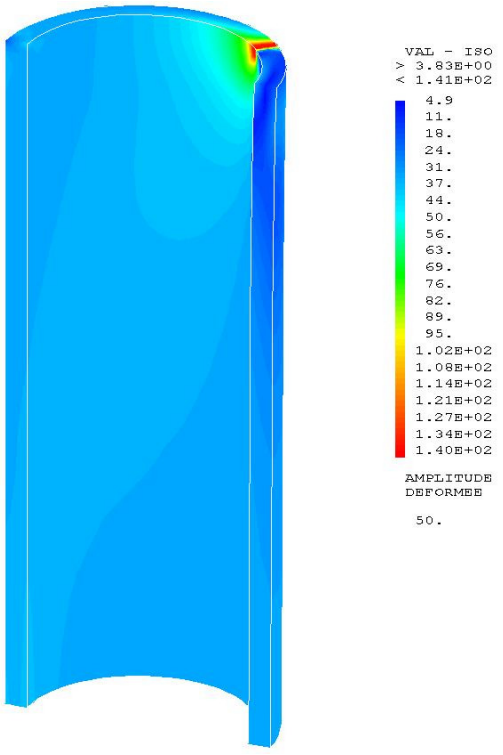


Figure 2.17
Von Misses stress distribution

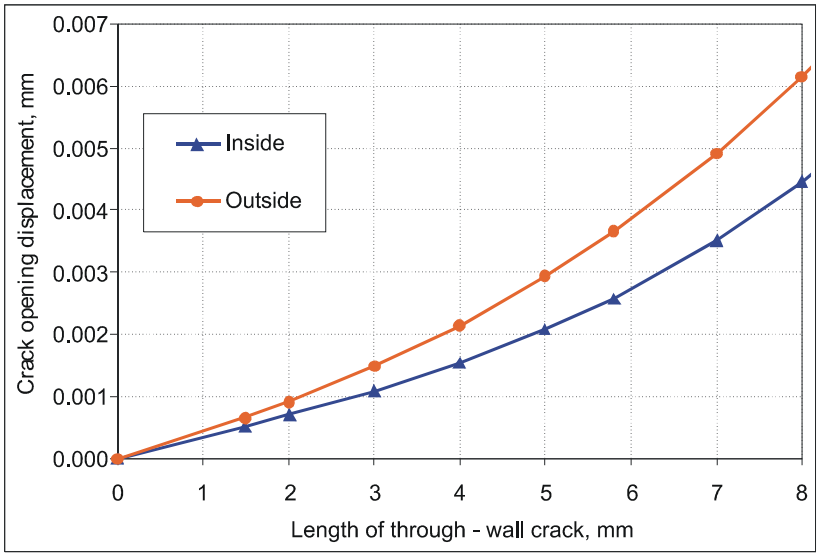


Figure 2.18
Crack opening function

two times less compared to critical crack length (6.5 mm). The target module 1H according to the used material properties complies with the LBB requirements.

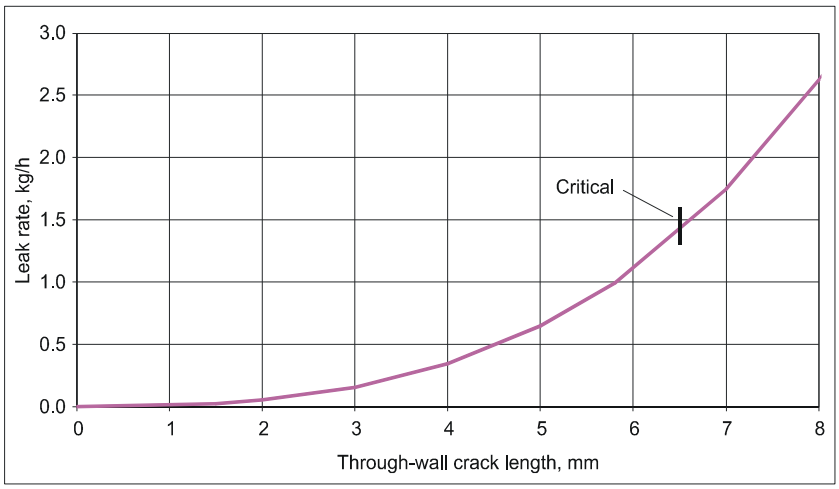


Figure 2.19
Variation of crack opening displacement with crack length

3 THEORETICAL INVESTIGATION OF ENERGY SPECTRA AND RELATIVE INTENSITIES OF RADIATION OF TUNGSTEN IONS

3.1 Development and usage of efficient computer codes for accurate calculations of spectral properties of W ions

A new quasi-relativistic Breit-Pauli approach consistent with the quasirelativistic radial orbitals has been formulated while fulfilling the tasks of the work plan 2008. All necessary computer codes have been created to calculate spectral characteristics within the approach. Applying the developed quasi-relativistic approach all the results are obtained by the configuration interaction method. The main stages of calculation are the following: first the quasi-relativistic Hartree-Fock equations are solved for the configurations under research; next the basis of the quasirelativistic transformed radial orbitals are created to describe the virtual excitations; further all possible admixed configurations within the created basis are investigated and only those configurations are selected which influence the wave functions of the configurations under research most of all; when the basis of admixed configurations is created the energy operator matrices are formed and diagonalized; then the energies of the levels and their eigenfunctions obtained by diagonalizing are used to calculate the characteristics of the electron transitions.

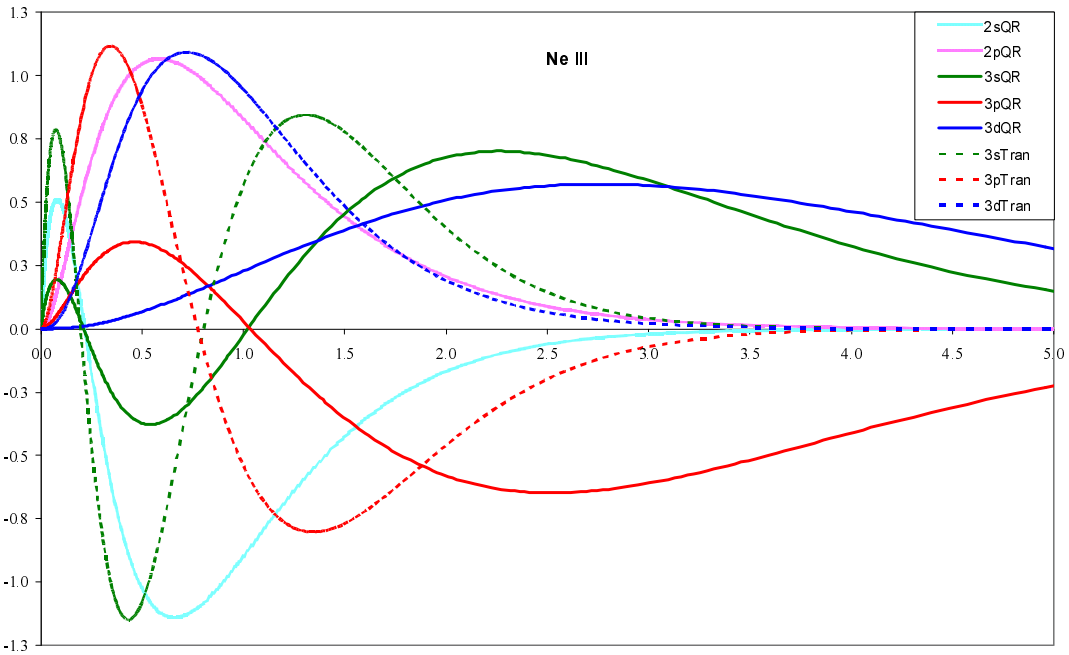


Figure 3.1
Quasi-relativistic radial orbitals of active shells 2s and 2p and radial orbitals with n=3 for configuration interaction – solution of quasi-relativistic equations (QR) and transformed radial orbitals (Tran)

The quasi-relativistic energy operator fully corresponds to the operator of the usual Breit-Pauli approach: besides the non-relativistic interactions all relativistic corrections to the order of the square of the fine-structure constant ¡ are calculated.

The effectiveness of the created approach have been tested while calculated the spectral characteristics of the highly charged ions Ne^{4+}, Fe^{18+}, Fe^{20+}, Ni^{20+} Xe^{41+} and others. All performed calculations confirmed the efficiency and high accuracy of the created quasi-relativistic approach. The obtained theoretical results are in excellent agreement with the experimental data much better than the ones obtained within the usual Breit-Pauli approach. It is achieved by taking into account the relativistic effects already when calculating the quasirelativistic radial orbitals and also by calculating efficiently the correlation corrections. The influence of the latter is taken into account employing the configuration interaction on the basis of the transformed radial orbitals.

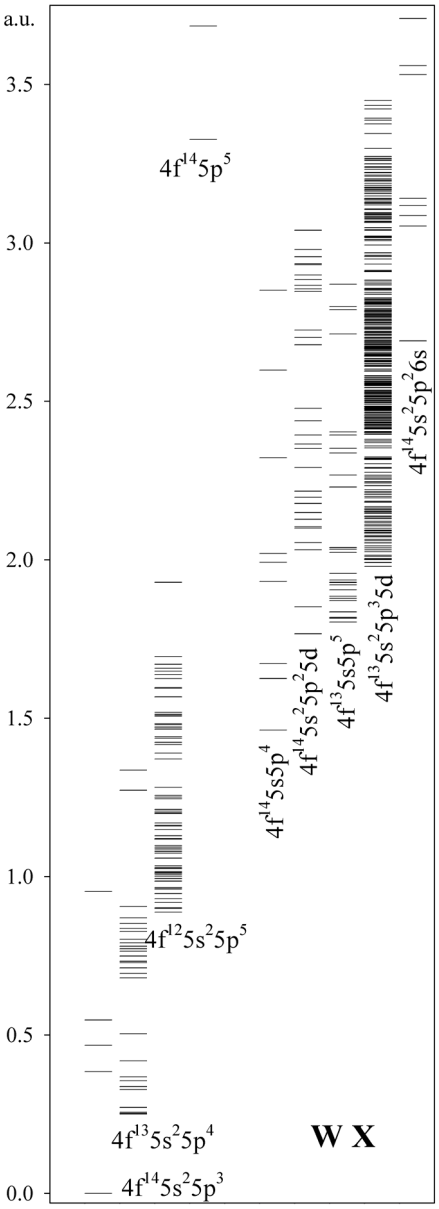


Figure 3.2
Energy spectra of W X calculated within quasirelativistic approach

These radial orbitals are very effective for description of the virtual electron excitations, since for these electrons the maxima of the transformed radial orbitals are much closer, comparing to the solutions of the quasirelativistic equations, to the maxima of the adjusted functions. The features of the transformed radial orbitals are clearly seen in Figure 3.1. In the figure the radial orbitals of active shells 2s and 2p of Ne III ion are plotted. Two possible types of radial orbitals with n=3 for configuration interaction are also presented – solution of quasi-relativistic equations (denoted QR) or quasi-relativistic transformed radial orbitals (denoted Tran).

The characteristics not only of quite simple and well-examined ions but also of various tungsten ions have been investigated using the created quasirelativistic approach. The spectral characteristics tungsten ions have been calculated using the usual Breit-Pauli approach as well.

While investigating the tungsten ion W^{9+} the energy spectra of two groups of configurations were calculated. The first group is composed of the ground configuration $4f^{14}5s^25p^3$ and other odd configurations $4f^{13}5s^25p^4$, $4f^{12}5s^25p^5$, $4f^{14}5p^5$; the second – of even configurations $4f^{14}5s5p^4$, $4f^{14}5s^25p^25d$, $4f^{13}5s5p^5$ and $4f^{13}5s^25p^35d$. The configurations of both groups are energetically close and strongly mixed except of $4f^{14}5p^5$ configuration, the energy of which is much bigger than of other odd configurations. The levels of this configuration are higher than the ones of the even configurations and there are no emission transitions from the even configurations under research to this configuration. Since the levels of all mentioned even configurations are within one region, their wave functions are strongly mixed. It makes identifications of the levels are complicated task. The calculated energy spectra of W^{9+} are presented in Figure 3.2. The same configuration mixing effects are obtained as in the case of highly charged tungsten ions (W^{29+} – W^{34+}) investigated in works of the year 2007. Furthermore, investigation of the energy spectra of W^{9+} is very complicated and time consuming due to open 4f-shells within the excited configurations. Thus not only the personal computers but also the possibilities offered by BalticGrid facilities have been used for calculations. Due to very big number of the levels of excited configurations with open 4f-shells and due to the strong mixing of the configurations the transition

characteristics can be calculated only essentially improving the used program complex and performing new calculations within Grid.

While investigating the energy spectra of the neutral tungsten W the even configurations $5d^46s2$, $5d^56s$ and $5d^6$, and the odd ones $5d^36s^26p$, $5d^46s6p$ and $5d^56p$ have been analyzed. Here an unexpected problem occurred. Solving of usual Hartree-Fock equations failed for excited electrons using the well-known computer code written by other authors. The solutions describing the electrons of the investigated configurations have been obtained using the computer code for solving the quasi-relativistic Hartree-Fock equations. So the spectral characteristic of the neutral tungsten are obtained within the quasi-relativistic approach only.

Three even $5d^46s$, $5d^5$, $5d^36s^2$ and three odd $5d^46p$, $5d^36s6p$, $5d^26s^26p$ configurations have been investigated for single ionized tungsten ion. While investigating this tungsten ion within the usual Breit-Pauli and the quasirelativistic approaches it has been shown that applying the quasirelativistic radial orbitals allows one to obtain much more accurate theoretical energy spectra. Within the usual Breit-Pauli approach even taking into account the correlation corrections explicitly the obtained ground configuration of W^+ is $5d^5$ though the experimental data shows ground level $5d^4(^5D)6s\ ^6D_{1/2}$. When performing the calculations within the quasi-relativistic approach the obtained ground level and the energies of the first excited levels are in good agreement with the known experimental data. It confirms that the created quasi-relativistic approach is reliable and allows one to improve the results not only for the highly charged ions but also for the heavy neutral atoms and their first ions. The transition characteristics have also been calculated. The obtained energy spectra of W^+ are presented in Figure 3.3.

The obtained scientific results are published in two articles [13, 14] and presented at two international conferences [15, 16].

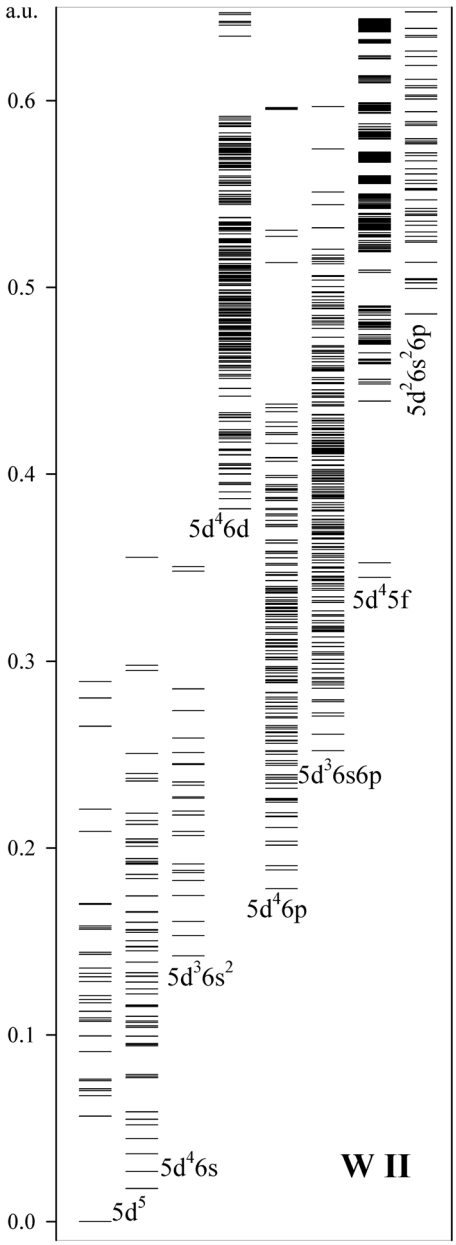


Figure 3.3 Energy spectra of W II calculated within quasirelativistic approach

3.2 Electron-impact double ionization of tungsten atoms and ions at low ionization stages

Some contribution to the production of the tungsten ions in plasma can be given by the cascade of Auger transitions after the single ionization of an inner shell. Such process is not yet considered in the database ADAS. According to the initial plan the modelling for ion charge distribution following inner shell ionization in the second and third ions of tungsten had to be performed. However, the investigation revealed that it was necessary to extend the number of considered ions, as well as to include the neutral tungsten. Additionally it was essential to take into account the direct many-electron ionization of ions. Thus the calculations have been performed for the neutral W and its ions W^{2+}, W^{4+} and W^{6+}, but this investigation has been limited by the first step of cascade, i.e. by the double ionization of ions.

The double ionization of tungsten ions at low ionization stages was measured and described by the semi-empirical formula [17], but no ab initio calculations were made. In our work the direct single ionization cross section has been calculated in the relativistic distorted wave or binary-encounter-dipole approximations; the contribution from the indirect ionization by the excitation-autoionization process was included too. After the single ionization of 4d, 4f, 5s and 5p shells some states can decay by the Auger transitions into the states of ions with one and two higher ionization stages. While such transitions take place between the neighbouring or overlapping configurations the detailed level-by-level calculations have been performed in the relativistic configuration interaction approximation using Flexible Atomic Code [18]. The direct double ionization of ions has been considered as a two step process: the initial single ionization by electron impact and the additional ionization due to a sudden perturbation of electronic shells. The contributions from the Auger transitions and from the sudden perturbation to the double ionization cross section are of the same order, though the last process plays a smaller role, especially for the higher ions. The calculated cross sections correspond approximately to the experimental data (Figure 3.4), probably, the difference is due to a less accurate calculation of direct double ionization using sudden perturbation model. Our results have been presented for publication [19].

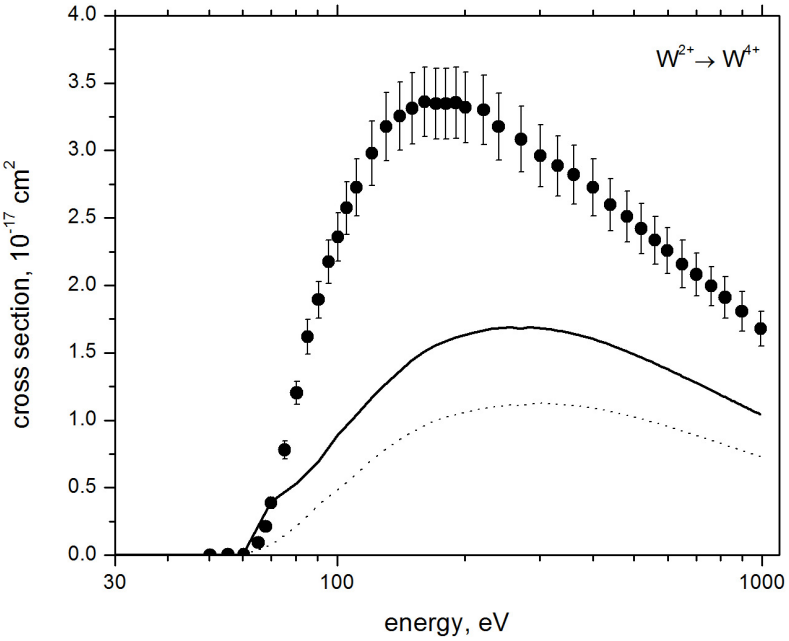


Figure 3.4
Cross sections for the electron-impact double ionization of W^{2+} ions. Results of calculations: bold line – total double ionization cross section; dotted line – double ionization without contribution of sudden perturbation process. Full circles with error bars show the results of experiment [13]

3.3 Theoretical investigation of the quenching of intensity in the 4d -4p and 4f - 4p transitions due to configuration mixing in the ions with 4d open shell

One of the most intense features emitted by tungsten ions from ASDEX Upgrade plasmas is the quasi-continuum band around 5nm [20]. It was interpreted in [21, 22] as corresponding to transitions ($4p^5 4d^9 + 4p^6 4d^7 4f$) – $4p^6 4d^8$ in W^{29+} W^{37} ions with the open 4d shell. Some regularities of the formation of this band were formulated in [23]. The aim of this work was to continue the theoretical investigation of the quenching of intensity in the narrow interval of wavelengths for these ions of tungsten. In order to establish the general conditions of this effect the variation of such band in isoelectronic sequences has been considered too.

At first it was approved the assumption that the integral characteristics of the intense group of lines were mainly determined by the interaction of only two strongly mixing $4p^5 4d^{N+1}$ and $4p^6 4d^{N-1} 4f$ configurations. Such assumption was suggested in [24] on the ground of calculations for the emission spectrum of only one W^{30+} ion. In this work the calculation using a large set of configurations has been performed for the emission spectrum of the W^{31+} ion and the same conclusion obtained. In both cases the calculated average wavelength of quasi-continuum band corresponds well to its experimental value.

It was shown that the concentration of intensity in a narrow interval of wavelengths mainly depends on the mutual positions of the levels of $4p^5 4d^{N+1}$ and $4p^6 4d^{N-1} 4f$ configurations which are mainly populated by the excitation from the ground level. When such levels of $4p^5 4d^{N+1}$ configuration are lying below the similar levels of $4p^6 4d^{N-1} 4f$ configuration, the emission spectrum is concentrated in a narrow interval of wavelengths. On the other hand, when some strongly populated levels of $4p^5 4d^{N+1}$ configuration are situated above or between such levels of $4p^6 4d^{N-1} 4f$ configuration, the transition array is less influenced by configuration interaction and the intensive lines are distributed in a wide interval. Such regularity is fulfilled in the isoelectronic sequences too.

The similarity of emission and photoexcitation spectra of tungsten ions noticed in [21] has been explained as a result of suppression by the configuration interaction of transitions to all levels of $4p^6 4d^N$ configuration except the ground level. These results have been presented for publication [25].

3.4 Relativistic methods for electron-ion scattering calculation

The emission-line spectra used for the plasma diagnostics, the energy losses due to plasma impurities are determined by solving the balance equation for the level populations of the ions in the different ionization stages. A detailed knowledge of the accurate atomic parameters describing the atomic structure (energy levels, radiative transition rates, Auger rates) and photon or charged particle scattering from ionized atoms is paramount for the construction of the balance equation. Theoretical methods to obtain scattering parameters are very complicated, especially when dealing with heavy and highly-charged ions. Consequently, one needs the sophisticated theoretical methods allowing simplifying the calculations and reducing the computing time required for a large scale data generation.

There exist quite a few methods to calculate the cross sections necessary for practical applications. One of the most accurate technique being the R-matrix method which includes nearly all the physical effects that contribute to cross sections and can be applied to all kinds of atoms, from neutral to highly ionized stages. Unfortunately, those calculations are prohibitively large and time consuming if performed in the relativistic coupling using a standard Dirac-Fock R-matrix method because the accuracy of obtained results depends on the number of target levels included (which is significantly larger comparing to a non-relativistic LS- term case). Therefore the methods based on transformation of the scattering matrices, calculated in the pure LS- coupling, to an intermediate coupling help to overcome the problem by reducing the number of terms. But the non-relativistic wave functions, used in the LS- coupling, become unsuitable to describe the highly-charged heavy ions where it is extremely important to use the relativistic wave functions.

We employ the approach based on the analogues of relativistic integrals allowing exploiting the relativistic wave functions obtained in Dirac-Fock approximation. The aim of the research is:

- to assess different methods in the relativistic R-matrix approach for electron scattering calculation, involving the highly-charged tungsten ions;
- to estimate the importance of correlation and relativistic effects in the case of the electron-impact excitation from the outer shell of heavy ions.

For this purpose we have determined the collision strengths Ł and the effective collision strengths of the electron-impact excitation to the levels of the configurations with one electron in the outer 4p, 4d, 4f, 5s, 5p, 5d, 5f, 5g, 6s, 6p, 6d, 6f, 6g shells from the ground state $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s$

(J = 1/2) and from some levels of the n = 4 configurations of the W^{45+} ion. In these calculations we have applied three different approaches to include the relativistic effects: 1) a standard Dirac-Fock R-matrix method (as implemented in the DARC code), 2) our method employing the analogues of relativistic integrals together with non-relativistic R-matrix code, and 3) the relativistic distorted wave approximation.

The extended basis of relativistic wave functions based on Dirac-Fock type radial orbitals was obtained at the beginning. These wave functions were determined for the ground state and for the excited states with outer electron in 4l, 5l′, 6l″, 7l‴ shells of the W^{45+} ions when l = 0,1,2,3; l′ = 0,1,2,3,4; l″ = 0,1,2,3,4,5; l‴ = 0,1,2,3,4,5,6. Using the obtained wave functions, we have calculated the energy level spectra in a completely relativistic Dirac-Fock approach applying configuration interaction (CI) method. This calculation includes the 93 energy levels with nd″ 7. The levels obtained in our calculation are presented in the following Figure 3.5.

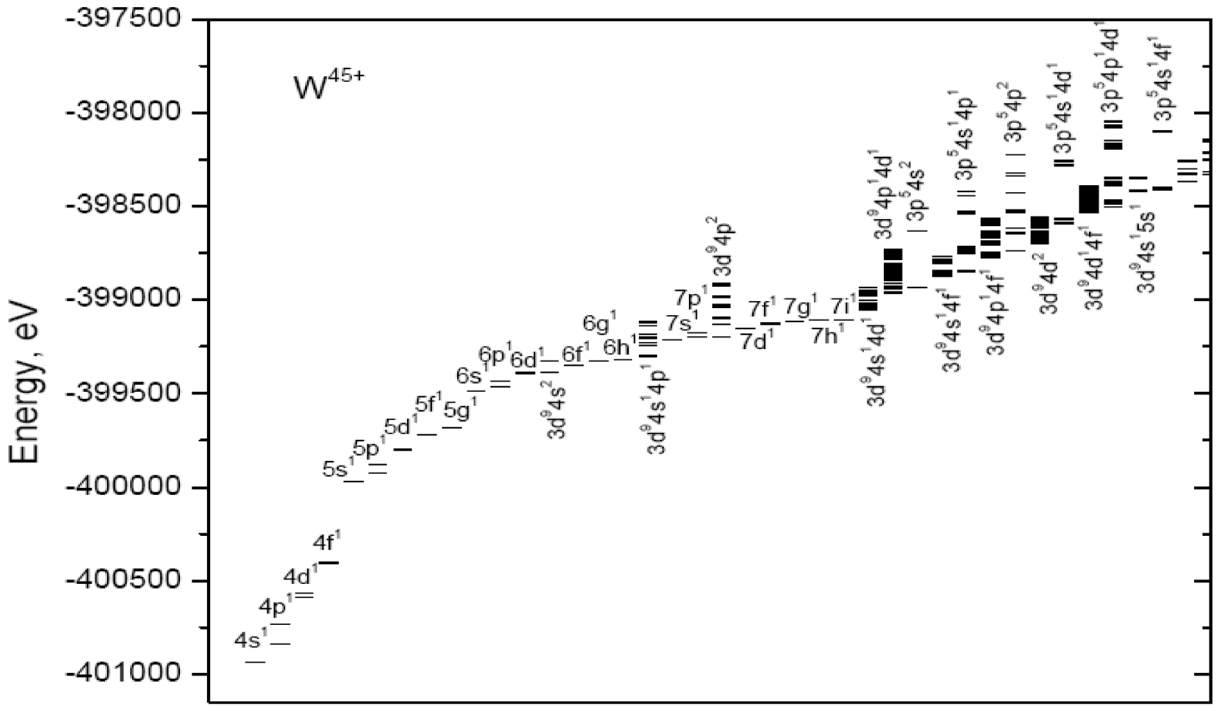


Figure 3.5
The energy level spectra in a completely relativistic Dirac-Fock approach of W45+ ions

To assess the accuracy of the computed wave functions, we have compared our energy levels determined using well-established relativistic atomic-structure package GRASP with other theoretical data and existing experimental results. We have found that our data are in a good agreement with experiment. Therefore we can assume that we have established wave function basis for the further calculation of scattering data and, consequently, are able to proceed with the calculation of collision strengths for the W^{45+} ions.

The non-relativistic R-matrix code that uses the relativistic analogues of integrals has been extended for the general case, which allows applying it for the configurations under consideration. Electron-impact collision strengths were calculated in the relativistic distorted-wave approximation using FAC suite of codes providing the base-line scattering data for the further comparison. The relativistic R-matrix calculations employing the regular scattering codes from the DARC program were performed, serving as a benchmark point for the comparison with the data, obtained from the non-relativistic R-matrix method based on the multichannel quantum defect theory and

intermediate coupling frame transformation. The electron-impact excitation collision strengths obtained with non-relativistic wave functions for the transition $4s_{1/2} - 4p_{1/2}$ in the W^{45+} ions is presented in Figure 3.6 below. Here we included only one-electron excitations in the n = 4 complex. As well relativistic DW calculations are shown to see the accuracy of methods for the highly charged tungsten ion. It is evident that the agreement of all data is good.

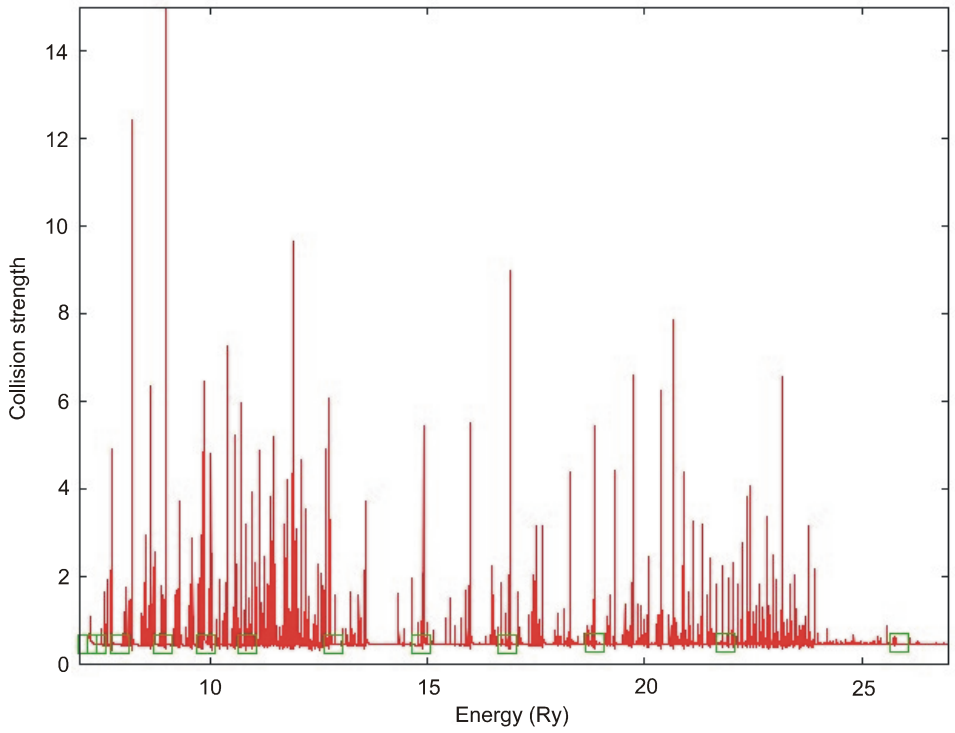


Figure 3.6 The electron-impact excitation collision strengths obtained with non-relativistic wave functions for the transition $4s_{1/2} - 4p_{1/2}$ in the W^{45+} ions

3.5 Properties of Auger electrons following excitation of polarized atoms by polarized electrons

Excitation of atoms by electrons is one of the most important processes in laboratory and astrophysical plasmas. The excited atom can 'remember' the direction and the polarization of the incident electron or photon and the following Auger electron may have a non-isotropic angular distribution. The main purpose of the present work [26] was to obtain the most general expression for differential cross section describing the properties of Auger-electron emission induced in the excitation of polarized atoms by polarized electrons. The special cases of this expression suitable for the interpretation of various experimental results can easily be derived. It is assumed that the probability of radiative decay is much smaller than that of the autoionization, and the isolated excited state with well defined total angular momentum is formed. This resonance state then autoionizes in the second step to some ionic state by emitting an electron.

The general expression for the cross section describing the Auger decay following the excitation of polarized atoms by polarized electrons was obtained for the first time in such collisions in which the two step approximation can be applied. The expression describes the polarization states and angular distributions of all particles in both the initial and final states. The cross sections for some special cases, i.e. the angular distribution of the Auger electrons following excitation of non-polarized atoms by-non polarized electrons, the angular correlations between the Auger and scattered electrons following excitation of non-polarized atoms by non-polarized electrons, and the magnetic dichroism in the angular distribution of the Auger electrons following excitation of polarized atoms by non-polarized electrons are derived to demonstrate the applications of the general expression for specific experimental conditions.

4 THE ACTIVITIES ACCORDING TO JET ORDER AND JET NOTATION

Two scientists from the Institute of Theoretical Physics and Astronomy of Vilnius University worked at JET. Dr. Valdas Jonauskas visit to UKAEA/Fusion, Culham, UK took place on July 20 – August 1, 2008. The following main aims were achieved during the visit:

- The calculated ion yield data after processes of Auger cascade in tungsten ions W^{2+}, W^{4+}, W^{6+} were discussed and decided to extend calculations to neutral tungsten.
- On the results of the previous calculations it was shown that shake-off processes can be important for the number of the doubly ionized ions. Shake-off processes would increase the yield of those ions.
- It was decided to extend ADAS database by double ionization rates from Auger cascade calculations in tungsten ions.
- Calculations of the wavelengths of radiative transitions for tungsten ions were presented when massive multiconfigurational calculations had been used and the mixing configurations had been obtained from CI (configuration interaction) strength.

Dr. R.Kisielius visit to EFDA-JET, Culham, UK took place on November 30 – December 11, 2008.

During this visit, the following tasks were achieved:

- The calculation results of the magnetic-dipole transitions in highly charged tungsten ions from W^{29+} to W^{37+} were presented and discussed.
- The methods to determine electron-impact excitation data for the W^{45+} ions by employing both the relativistic program package DARC and our derived method of the analogues of relativistic integrals were discussed and the comparison of the results was presented.
- The Flexible Atomic Code program package was installed on JET computer cluster. The initial calculation of the energy levels of W^{13+} and W^{14+} ions was performed and the results were presented.
- The possibilities to study the parameters, including energy levels, Auger transition rates and dielectronic recombination rates, of the autoionizing states of W^{13+}, W^{14+}, W^{7+} and W^{8+} were discussed and the preliminary calculations were performed.

5 THE ACTIVITIES IN SOCIO-ECONOMIC STUDIES

LEI intention in Socio-Economic research field is to contribute to the development of the EFDA word energy model for evaluation of effectiveness of nuclear fusion plants and evaluation of their economic effectiveness in the Baltic region.

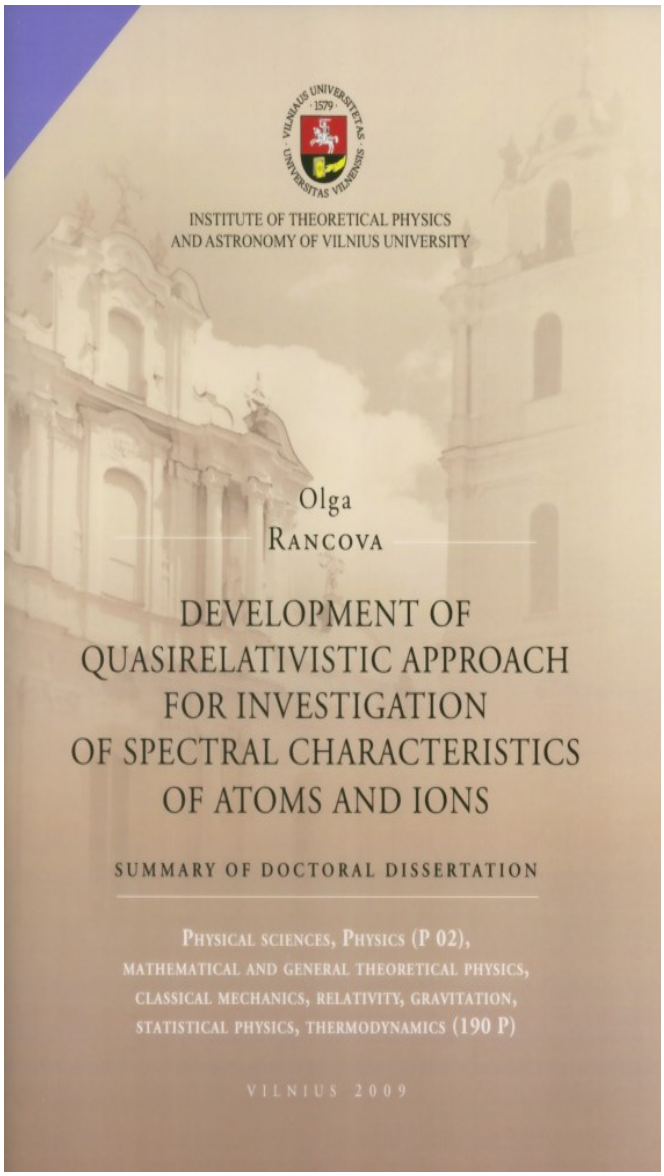
The structural changes are needed in the existing EFDA TIMES module representing the Former Soviet Union (FSU) and Eastern European Union (EEU) regions. In particular, there is a need of separation of new EU member countries from the TIMES module representing the Former Soviet Union and their integration into EEU module. Collection of information representing energy sector of the Baltic countries (Estonia, Latvia, and Lithuania), as well as preparation of mathematical model for energy systems of the Baltic countries and evaluation of economic efficiency of fusion power plants for satisfying energy demand of the region can be performed by the LEI experts.

In May 2008 a call was received for participation in Socio-Economic Studies. However, the FUSION model application for FSU and EEU regions is not foreseen within the Studies to be performed under this Call. Therefore, actual LEI activity in this field has not been started yet.

6 TRAINING AND EDUCATION

A series of lectures „Joint Research Centre: Science – industry – product – user – science" were held for the scientists and students at the Institute of Theoretical Physics and Astronomy of Vilnius University. A lecture about the news in thermonuclear fusion and reactor was given by Jef Ongena (the European Commission).

The doctoral dissertation by O. Rancova "Development of quasirelativistic approach for investigation of spectral characteristics of atoms and ions" was prepared with acknowledgement of the support of the project. The dissertation was defended on January 8, 2009.



7 MOBILITY PROGRAM 2008

Mr. Valdas Jonauskas participated in the EFDA Diagnostics Work Programme 2008/2009 meeting, which was held on March 5-6, 2008 in Garching, Germany.

According to work programme item 1.4 “Power and particle exhaust and plasma-wall interaction” two missions were organised to UKAEA Culham.

Dr. V. Jonauskas visit to UKAEA/Fusion, Culham, UK took place on July 20 – August 1, 2008. The following main aims were achieved during the visit:

- The calculated ion yield data after processes of Auger cascade in tungsten ions W^{2+}, W^{4+}, W^{6+} were discussed and decided to extend calculations to neutral tungsten.
- On the results of the previous calculations it was shown that shake-off processes can be important for the number of the doubly ionized ions. Shake-off processes would increase the yield of those ions.
- It was decided to extend ADAS database by double ionization rates from Auger cascade calculations in tungsten ions.
- Calculations of the wavelengths of radiative transitions for tungsten ions were presented when massive multiconfigurational calculations were used and the mixing configurations were obtained from CI (configuration interaction) strength.

Dr. R. Kisielius visit to EFDA-JET, Culham, UK took place on November 30 – December 11, 2008.

During this visit, the following tasks were achieved:

- The calculation results of the magnetic-dipole transitions in highly charged tungsten ions from W^{29+} to W^{37+} were presented and discussed.
- The methods to determine electron-impact excitation data for the W^{45+} ions by employing both the relativistic program package DARC and our derived method of the analogues of relativistic integrals were discussed and the comparison of the results was presented.
- The Flexible Atomic Code program package was installed on JET computer cluster. The initial calculation of the energy levels of W^{13+} and W^{14+} ions was performed and the results were presented.
- The possibilities to study the parameters, including energy levels, Auger transition rates and dielectronic recombination rates, of the autoionizing states of W^{13+},W^{14+}, W^{7+} and W^{8+} were discussed and the preliminary calculations were performed.

According to work programme item 4.7 “Fusion safety issues” there were organised two missions to IPP Greifswald. Missions were organised on June 23–28, 2008 and December 1–6, 2008. During the first mission 3 experts from LEI – Mr. Dundulis, Mr. Kaliatka, and Mr. Urbonavicius visited IPP Greifswald to discuss the first approach to the modelling of W7-X. Detailed discussions regarding W7-X design and operation during “baking” mode were held. After these discussions it was agreed how the models developed at LEI for RELAP5 and COCOSYS codes should be updated to consider the peculiarities of W7-X “baking” and main cooling circuits.

As well during this mission the finite element model of the target modulus for stress analysis and selection of most loaded part were presented. It was agreed to perform the leak before break analysis for the most loaded component. The comments for presented model were received and they will be evaluated in developing this model. Together with Mr. Naujoks of IPP there were discussed questions about the material properties and fracture parameters for leak before break analysis of target modulus. IPP will provide the material properties of the target modulus steel. LEI will select the fracture parameters of stainless steel from own experiences for crack analysis.

On December 1–6, 2008 the visit of the LEI experts to IPP took place. Purpose of this visit was to discuss obtained calculation results and to update available project data. During the visit W7-X facility and installed piping were shown around. Besides, obtained calculation results were thoroughly discussed and missing data was identified. Moreover, work program for the year 2009 was discussed.

Task Force PWI Meetings

No participation in PWI meetings in 2008.

LEI representatives G. Dundulis (on the left) and T. Kaliatka (in the center) discuss details of the W7-X device with the IPP representative D. Naujoks (on the right)

LEI representative E. Urbonavičius (on the left) discuss obtained calculation results with IPP representative D. Naujoks (on the right)

8 PUBLIC INFORMATION

The information related with FUSION energy perspectives, last achievements in ITER development and other Fusion research fields is continuously distributed among universities, R&D institutions, schools:

- Occasionally school teachers (physics, chemistry …) from various regions of Lithuania visit the Institute. In addition they receive information and brochures on fusion. Information is spread via personal contacts as well.
- Through our partner Vytautas Magnus University, which is located in Kaunas, Lithuania, the information is spread to schools when university looks for students to physics studies.
- 14th March 2008. "Career days" at Kaunas University of Technology, Kaunas Lithuania. Distribution of information on FUSION to students.
- 14th May 2008. "Carrier days" at Vytautas Magnus University, Kaunas, Lithuania. Distribution of information on FUSION to students.
- 24th May 2008. 6th International Exposition "Kaunas 2008", Kaunas, Lithuania, devoted to 600 years of Kaunas. Distribution of information on FUSION to public.
- 29th May 2009. 5th Conference of young scientists on energy issues CYSENI 2008 (www.cyseni.com). Conference is with regional (Estonia, Latvia, Lithuania, Belarus, Russia) attention. In the conference "Fusion energy" topic is included (1 of 11). Two papers were presented at the conference.

Three lectures "We can produce energy as stars do it" have been presented by O. Rancova to the general public within the framework of European Researchers' Night on September 26, 2008. ITER project and participation of Lithuanian scientists in it were introduced by the lecturers.

9 PUBLICATIONS

9.1. P. Bogdanovich and O. Rancova, Quasirelativistic approach for ab initio study of highly charged ions Physica Scripta, v. 87 (2008) 045301 (9pp).

9.2. O. Rancova, P. Bogdanovich and R. Karpuškienė, Quasirelativistic ab initio study of Gallium like Molybdenum and Tungsten J Phys, Conf ser. (in press).

9.3. O. Rancova, P. Bogdanovich and R. Karpuškienė, Application of new quasirelativistic approach for treatment of oxygen-like Iron and Nickel 40th EGAS Conference, Graz, 2008, Abstracts, p. 43.

9.4. P. Bogdanovich, O. Rancova and R. Karpuškienė, Quasirelativistic ab initio study of galium-like molibdenum and tungsten, 14th International Conference on the Physics of Highly Charged Ions, HCI2008, Tokyo, Japan, Book of Abstracts, p. A-a10.

9.5. V.Jonauskas, S.Kučas and R.Karazija. Electron-impact double ionization of tungsten atoms and ions at low ionization stages, Phys. Scr. (submitted).

9.6. S. Kučas, R. Karazija, V. Jonauskas, and A. Momkauskaitė. Interaction of $4p^5 4d^{N+1}$ and $4p^6 4d^{N-1} 4f$ configurations and their influence on the photoexcitation and emission spectra in the isoelectronic and isonuclear sequences (submitted).

9.7. A. Kupliauskienė, V. Tutlys. Properties of Auger electrons following excitation of polarized atoms by polarized electrons, Nucl. Instr. Meth. Phys. Res. B, **267**, 263 (2009).

9.8. Kačegavičius T. Development of fusion facility W7-X model for ASTEC code // 5th conference of young scientists on energy issues CYSENI 2008, Kaunas, Lithuania, 29 May, 2008. Kaunas: LEI, 2008. ISSN 1822-7554, p. 1-10. [INSPEC]

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10 IMPLEMENTATION OF QA SYSTEM

The quality assurance system according to standard LST EN ISO 9001:1995 requirements in Lithuanian Energy Institute was developed in 1999.

In 2001 the updating of quality assurance system of institute on the basis of requirements of standard LST EN ISO 9001:2001 was initiated. According to these requirements the quality package of quality assurance documents in LEI was developed.

On February 17, 2004 the quality system of institute is certified by the Lithuanian Standards Board under the Ministry of Environment of the Republic of Lithuania and the certificate of quality management system conformity to standard LST EN ISO 9001:2001 is received. On February 15, 2007 duration of certificate was extended for the next three years.

The safety analysis of FUSION facilities is included in the procedure "PA/17-02, Control of nuclear installation safety research process", which is prepared in accordance with LST EN ISO 9001:2001 standards and operating together with other LEI quality management system procedures.

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