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Neutronic and thermal-hydraulic coupling for 3D reactor core modeling combining MCB and fluent

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Abstract. Three-dimensional simulations of neutronics and thermal hydraulics of nuclear reactors are a tool used to design nuclear reactors. The coupling of MCB and FLUENT is presented, MCB allows to simulate neutronics, whereas FLUENT is computational fluid dynamics (CFD) code. The main purpose of the coupling is to exchange data such as temperature and power profile between both codes. Temperature required as an input parameter for neutronics is significant since cross sections of nuclear reactions depend on temperature. Temperature may be calculated in thermal hydraulics, but this analysis needs as an input the power profile, which is a result from neutronic simulations. Exchange of data between both analyses is required to solve this problem. The coupling is a better solution compared to the assumption of estimated values of the temperatures or the power profiles; therefore the coupled analysis was created. This analysis includes single transient neutronic simulation and several steady-state thermal simulations. The power profile is generated in defined points in time during the neutronic simulation for the thermal analysis to calculate temperature. The coupled simulation gives information about thermal behavior of the reactor, nuclear reactions in the core, and the fuel evolution in time. Results show that there is strong influence of neutronics on thermal hydraulics. This impact is stronger than the impact of thermal hydraulics on neutronics. Influence of the coupling on temperature and neutron multiplication factor is presented. The analysis has been performed for the ELECTRA reactor, which is lead-cooled fast reactor concept, where the coolant flow is generated only by natural convection.

Key words: code coupling • modeling • Monte Carlo • neutronics • nuclear reactor • thermal hydraulics

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Introduction

Nowadays, most sciencific projects are based or supported by computer modeling, which widely extends the scope of problems that can be addressed and solved. In the nuclear reactor research, supercomputers allow for three-dimensional simulations of neutronics and thermal hydraulics of reactor cores. Moreover, all considered phenomena are being analyzed simultaneously in an integrated model, yet allowing the user for consideration of many variables such as detailed part dimensions, properties of applied materials, and different boundary conditions. Data exchange between neutronics and thermal hydraulics is significant for correct modeling of reactor operation. Therefore, the development of systems that couple thermal hydraulics with neutronics is the aim of research at many institutions [1–5]. Such a coupling has been made also at AGH University of Science and Technology, where FLUENT [6], which is CFD code commonly used in industrial applications, is coupled with the MCB code [7], which serves neutronics and fuel cycle calculation. MCB – Monte Carlo continuous energy burnup code is a general-purpose code used to calculate a nuclide density time evolution including burnup and decay. MCB comprises internally MCNP code [8], which is used for transport calculations. The main purpose of the coupling is to exchange data between both processes: neutronics and thermal hydraulics. The temperature field inside the reactor core, which results from thermal calculations, is needed for neutronic calculations, because cross sections of nuclear reactions depend on the material temperature. The power density profile in the fuel obtained in the neutronic calculations is an input for the thermal calculations and then the resultant temperature distribution is feedback to the neutronic calculations. The effect of the coupling between neutronics and thermal hydraulics has been analyzed for case of ELECTRA reactor, which is a small lead-cooled fast reactor concept developed at KTH in Stockholm [9]. The flow of the coolant in the core is generated by natural convection, thus thermal hydraulics is crucial in that case. The verification of the calculations was performed with a code to code comparison using results obtained by scientists at KTH. Their thermal analysis was performed using SAS4A/SASSYS-1 code and numerical model has taken into account using only the simple model of a single fuel pin with adjacent coolant [10], whereas presented analysis was done for the full three-dimensional reactor core.

Setup

Simplified version of the European Lead-cooled Training Reactor (ELECTRA) shown in Fig. 1 was used in the analysis. Reactor core is in the center of the inner vessel. Six control barrels are located around the core. Each control barrel has two halves: the first one is a reflector whereas the second one is a moderator. Reactor power is controlled by rotation of the control barrels. Cold liquid lead flows down between the main and the inner vessel according with blue arrows, coolant is heated by the reactor core and flows up as the red arrow shows.

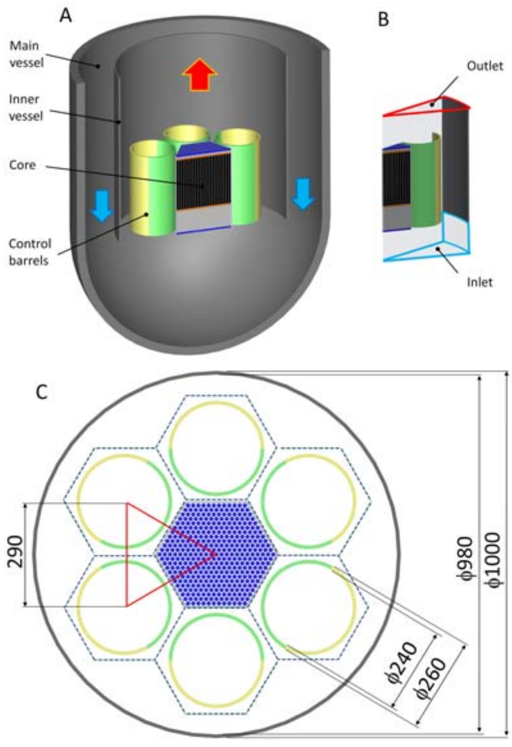

Fig. 1. Construction of ELECTRA reactor. Neutronic model (A, C), CFD model of reactor (B).

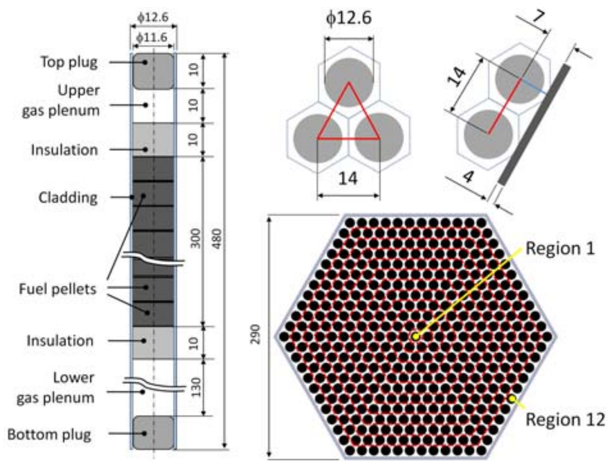

Fig. 2. Construction of fuel pin and reactor core. Division of the core into 12 radial regions. All dimensions in mm.

Two separate models have been performed for the coupled simulation: a neutronic model for MCB and a CFD model for FLUENT. The neutronic model comprises the whole reactor core including the main vessel with liquid lead, the CFD model shown in Fig. 1B includes only a part of the reactor core, which is defined by the symmetry of the core. The CFD model takes into account details that are not significant for the neutronics and therefore neglected in the MCB model.

Construction of fuel pins and their positions in the core are shown in Fig. 2. The reactor core includes 397 fuel pins and a steel wrapper around pins. Nominal operation of the reactor was analyzed and for that case, thermal power is 0.5 MW, that gives average power density in fuel roughly 39.7 MW/m^3. Fuel is based on (Pu,Zr)N since it has good thermal conductivity, it changes between 10 and 25 W/(mK) as a function of temperature. Percentage atomic fuel composition of Pu/Zr/N is as follows 20/30/50, whereas detailed atomic composition for Pu isotopes 238/239/240/241/242 is 4/52/24/12/8. Regarding the control barrels material, steel was used as the reflector, whereas steel with 47% of B_4C creates the moderator [10].

In order to simulate correctly the coolant flow, properties of liquid lead such as density, heat capacity, thermal conductivity, and viscosity were defined as functions of temperature [11]. Moreover, thermal conductivity of the fuel also changes with temperature in the numerical model since it strongly impacts on temperature gradient in the fuel pellets.

Regarding thermal-hydraulic settings, pressure outlet/inlet type of boundary condition with 400°C backflow temperature was set up on inlet/outlet surface and a pressure profile in the coolant volume as a function of height was defined to model natural convection. Prestudy of the coolant behavior shows that the flow is turbulent thus realizable k-epsilon

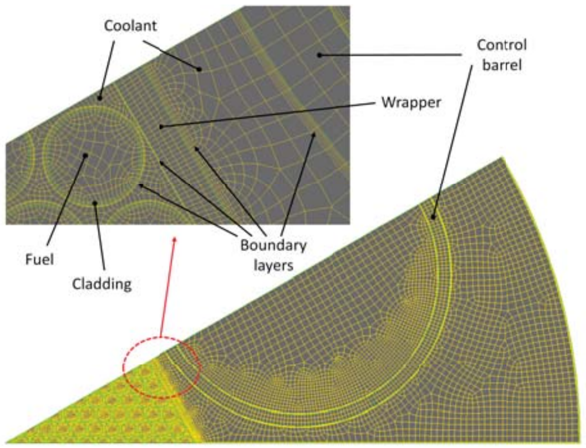

Fig. 3. Mesh for CFD numerical model of ELECTRA reactor core.

model with full buoyancy effects and enhanced wall treatment was applied. Additionally, standard *k*-omega model was investigated. As a source of heat, volume heat source in the fuel was fixed.

The geometry for thermal hydraulics was prepared using standard CAD software and exported to GAMBIT where a mesh was created for FLUENT. The mesh presented in Fig. 3 includes roughly 7.74 $\times 10^6$ elements, it is a structured mesh with several boundary layers around rods, wrapper and control barrel. Boundary layers include 2–4 layers with various thickness depending on their positions. Quality of the mesh was checked by functions dedicated for this purpose, which are available in GAMBIT. Mainly the skewness factor was used and its value for the mesh was below 0.7, it is good quality mesh.

In case of the neutronic simulation, most important particles such as neutrons and gammas were modeled in detail, whereas electron transport was simplified. Such an approach is appropriate for our investigation. Electrons are not tracked in detail since it increases the time of calculation. Prompt and delayed particles from fission as well as from activation are taken into account. Moreover, fuel burnup and transmutation of materials in time are included in the simulation. Neutron multiplication factor (*k*-eff) is calculated in specified points in a time. Simultaneously with the multiplication factor a power density profile in the fuel is computed.

Regarding nuclear cross sections, various libraries were investigated such as ENDF, JENDL, and JEFF. However, each library gives similar result in the case of ELECTRA reactor.

Coupling

The dedicated script was created by authors for the coupling, which executes FLUENT and MCB in the coupled simulation and allows to exchange data between both tools. MCB and FLUENT are not modified thus the script can work with each version of those codes.

The main purpose of the coupling is the data exchange between both processes: neutronics and thermal hydraulics, the scheme of the coupled simulation is shown in Fig. 4. MCB during transient neutronic simulation generates specific points in time. The power profile required for FLUENT and calculates other nuclear parameters. Obtained power profile is used by FLUENT in steady state heat and mass transfer simulation to compute the temperature field needed by MCB. Temperature is updated in the neutronic model and the transient neutronic simulation proceeds. Initial temperature for the neutronic simulation is computed using estimated power profile before MCB starts.

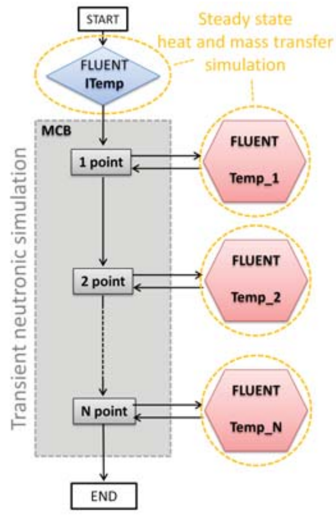

Fig. 4. Scheme of coupled simulation.

Regarding the data exchange, a fuel volume was divided into several smaller volumes to create a matrix of volumes, which represents whole fuel. The matrix describes a 3D profile of power density or temperature, that is used as an input and output during the data exchanging. To create the matrix, the fuel volume was divided into twelve radial regions, see Fig. 2. Additionally, each radial region includes several axial subregions to increase resolution of the power density profile and the temperature profile. Single volume of the fuel in specific axial and radial position is used to calculate average power density or average temperature, these quantities create matrix elements.

To investigate the influence of the data exchange, two noncoupled basic simulations have been performed. Basic CFD model assumes constant power density (39.72 MW/m^3) in the fuel, whereas basic neutronic model uses constant temperature in the fuel (900 K).

Results

The influence of the data exchange between neutronics and thermal hydraulics is presented. The data exchange impacts significantly on thermal hydraulics but has not strong influence on neutronics.

Comparison of the *k*-effective value evolution in time is presented in Fig. 5. Differences are negligible because in both simulations similar cross sections have been used. Cross-section libraries describing probabilities of nuclear reactions are prepared for

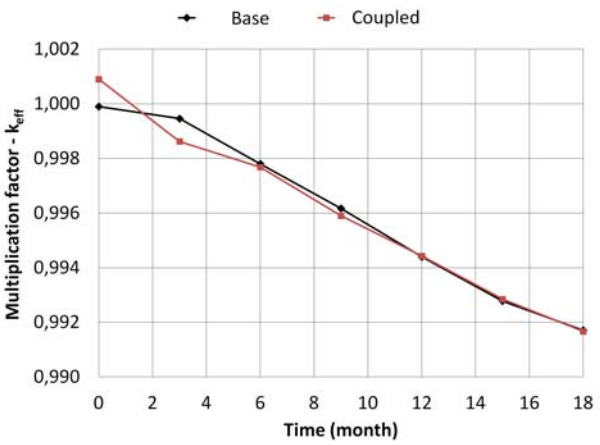

Fig. 5. Evolution of the *k*-effective value in time.

specific temperatures and temperature step between them is 100 K. In basic neutronic simulation, estimated fuel temperature is constant and equals 900 K thus only the cross section for 900 K is used. That temperature is close to the temperature field occurring in the reactor core, which was calculated in the coupled analysis. Table 1 shows the list of cross-section libraries used in the coupled analysis. Library 900 K, which was used in the basic simulation, was applied for 38.94% of the fuel in the coupled analysis. Mainly two libraries: 800 K and 900 K are used in the coupled simulation, differences between them are not significant thus the date exchange influence on neutronics is not strong.

The power profile shown in Fig. 6 is constant in time and differences between both the basic and the coupled case are not significant. The profile is constant because the investigated time is short thus the fuel composition does not change. Results from the basic and the coupled simulation are similar due to small differences between cross-section libraries. The maximum power factor located in the center of the active core is 1.6705, that gives roughly 67.36 MW/m³. Minimal value of the power factor is located in the periphery of the core and equals 0.5037, that is 20.00 MW/m³.

Table 1. List of cross-section libraries used in the coupled simulation for fuel

Fuel temperature [K]	Contribution of fuel volume [%]	Library
650–750	17.41	700
750–850	43.00	800
850–950	38.94	900
950–1050	0.65	1000

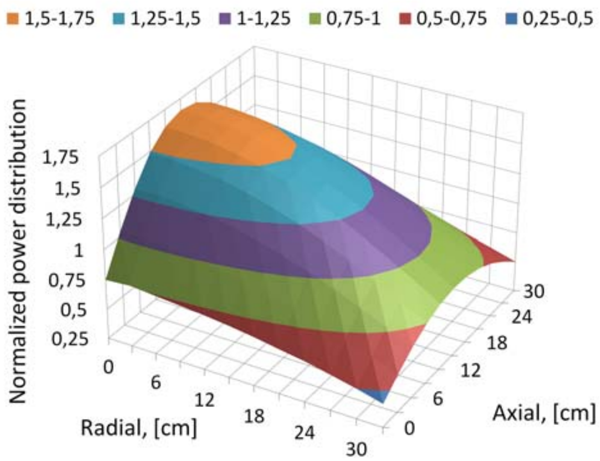

Fig. 6. Power profile in reactor core.

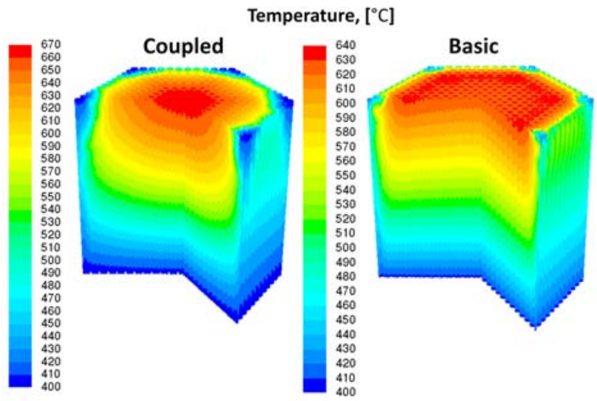

Fig. 7. Comparison of temperature fields in fuel.

Regarding thermal hydraulics, neutronics strongly affects on thermal behavior of the reactor. Maximum temperature in the fuel is 642.8°C and 683.6°C, respectively, for the basic and the coupled case, whereas the average temperature equals 527.2°C (basic) and 526.9°C (coupled). The maximal temperature in the coupled case is higher than in the basic case mainly due to high energy generation in the center of the core. Average temperature is similar because the temperature peak is compensated by lower temperature in the periphery.

Comparison of the temperature fields in the fuel is shown in Fig. 7. If the constant average power density in the fuel is used – the basic case, the hot spot is located at the fuel top in the 8th region. If the real power profile is applied, the hot spot is at the top of the fuel in the 1st region – the central pin. In both cases, we observe that the fuel in corners is cooled more efficiently. The fuel temperature in the center of core in the coupled simulation is higher than in the basic case because more energy is released in the center than in periphery. Moreover, the fuel located in periphery has lower temperature in the coupled case compared to the basic.

Fuel maximum temperature curves are shown in Fig. 8. The hot spot in both cases occurs at the top of the fuel. The hottest fuel pin in the coupled

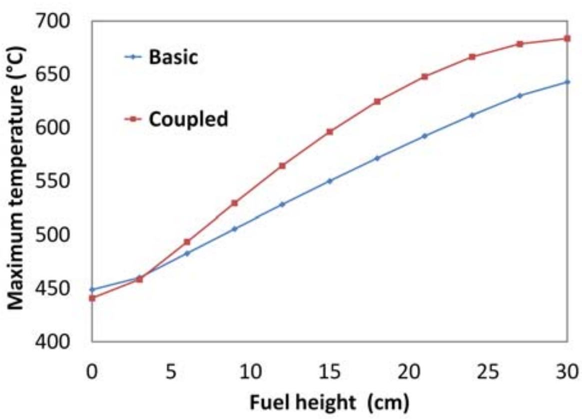

Fig. 8. Fuel maximum temperature.

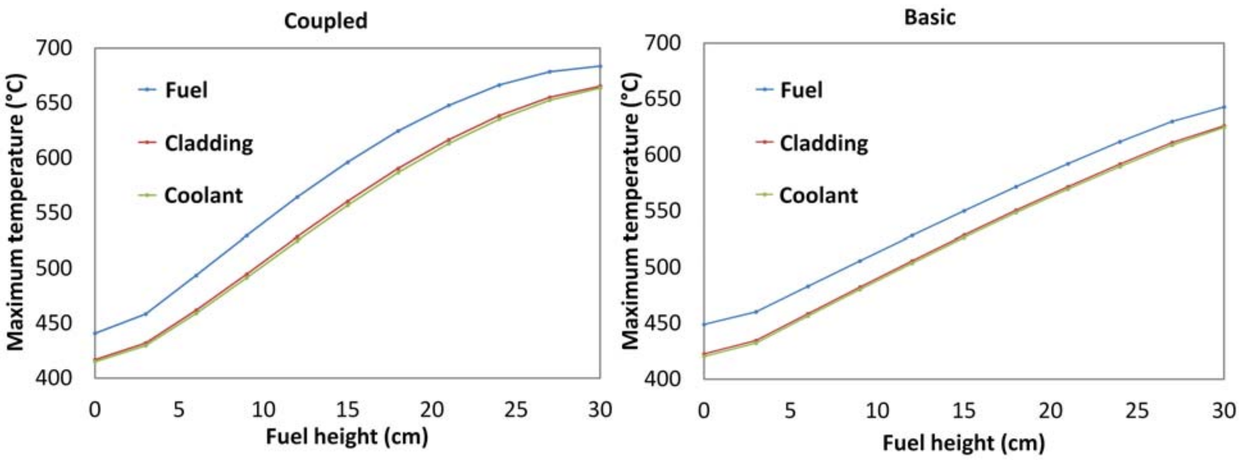

Fig. 9. Comparison of maximum temperature curves of fuel, cladding and coolant.

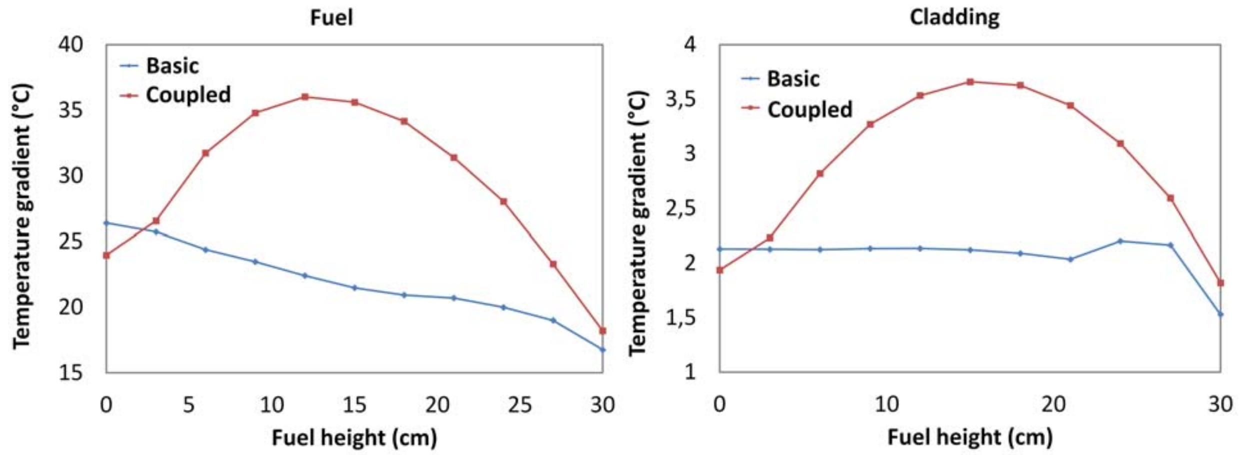

Fig. 10. Radial temperature gradient in fuel and cladding.

scenario is the central one, whereas in the basic case, pins in the 8th region have the highest temperature. Temperature in the coupled scenario is higher compared to the basic due to differences of power density in the fuel.

Figure 9 shows maximum temperature curves in the fuel, the cladding and the coolant. Fuel maximum temperature is located in the center of fuel pellets in the hottest fuel pin, maximum temperature in case of the cladding occurs on the contact between fuel pellets and the cladding. Obviously, the hottest coolant is on the outer cladding surface. We may observe gradient of temperature in the fuel pellets comparing the fuel curve to the cladding curve. To get the gradient of temperature in the cladding, we compare the cladding curve to the coolant curve.

The radial gradient of temperature in fuel and cladding is presented in Fig. 10. Temperature gradient in the basic case is lower and decreases with height, whereas in coupled case totally different behavior is observed. The gradient is higher in the center, where the power density is on a higher level. Similar situation is seen in the case of the temperature gradient in the cladding.

Conclusion

The coupling of neutronics and thermal hydraulics created by authors exchanges data such as the power profile and the temperature field in the reactor core between MCB and FLUENT. The power profile and the temperatures are required as an input for thermal and neutronic simulations. Estimated values of those parameters may be used. However, the application of the coupling is a better solution than assumption of estimated values of the temperatures or the power profiles since it allows to avoid mistakes associated with estimation of these parameters. The data exchange does not impact significantly on neutronics but the coupling may be used to check the temperatures needed to choose correct cross sections of nuclear reactions. Results show that the coupling is crucial for the thermal analysis since it depends significantly on the power profile, which defines the heat source and is strongly connected with nuclear reactions in the fuel.

Thermal hydraulics connected with neutronics gives valuable information about thermal reactor behavior, which is crucial for the reactor operation. The coupling allows to investigate the coolant flow, the temperature field, influence of the material properties on reactor operation, the power profile and the evolution of the fuel in time.

The coupled analysis will be applied to study IV generation reactors such as high temperature reactors (HTR) where helium gas is used as a coolant and graphite is a moderator. Moreover, the fuel transmutation can be analyzed since MCB code is capable of calculating changes occurring during fuel burnup.

References

1. Yan, Y., Rizwan-uddin, & Kim, K. (2008). *A coupled CFD-system code development and application*. PHYSOR, Interlaken, Switzerland.
2. Reiss, T., Fehér, S., & Czifrus, S. (2008). Coupled neutronics and thermo hydraulics calculations with burn-up for HPLWRs. *Progr. Nucl. Energy*, *50*, 52–61.
3. Seker, V., Thomas, J. W., & Downar, T. J. (2007). Reactor physics simulations with coupled Monte Carlo calculations and computational fluid dynamics. In Proceedings of International Conference on Emerging Nuclear Energy Systems (ICENES 2007).
4. Breitkreutz, H., Rohrmoser, A., & Petry, W. (2010). 3-Dimensional coupled neutronic and thermal-hydraulic calculations for a compact core combining MCNPX and CFX. *IEEE Trans. Nucl. Sci.*, *57*(6), 3667–3671.
5. Jianwei, Hu, & Rizwan-uddin. (2008). *Coupled neutronics and thermal-hydraulics simulations using MCNP and FLUENT. Advancements in multi--physics reactor simulation.* USA.
6. Fluent Inc. (2006). *FLUENT 6.3 User's Guide*. Fluent Inc.
7. Cetnar, J. (2006). *User Manual for MCB 5*. Kraków: AGH WFiIS.
8. *MCNP – A general Monte Carlo code n-particle transport code, Version 5*. (2008). X-5 Monte Carlo Team.
9. Wallenius, J. (2010). Lead cooled fast reactors. In Proceedings of LEADER Workshop on KTH Stockholm, Department of Reactor Physics.
10. Wallenius, J., Suvdantsetseg, E., & Fokau, A. (2011). *ELECTRA: European Lead cooled Training Reactor*. Stockholm: Reactor Physics, KTH.
11. Wallenius, J. (2010). Physical properties of lead. In Proceedings of LEADER Workshop on KTH Stockholm, Department of Reactor Physics.