

CFD analysis of the safety related thermal hydraulic parameters describing a flow domain of an experimental medical installation (BNCT converter) inside of the Research Reactor MARIA

Piotr Andrzej Prusiński^{*,a}, Sławomir Potempski^a, Mieczysław Borysiewicz^a, Karol Kowal^a, Tomasz Kwiatkowski^a, Andrzej Marcin Prusiński^b

^aNational Centre for Nuclear Research (NCBJ)
A. Sołtana 7, 05-400 Otwock-Świerk, Poland

^bInstitute of Heat Engineering, Warsaw University of Technology
Nowowiejska 21/25, 00-665 Warsaw, Poland

Abstract

The Boron-Neutron Capture Therapy (BNCT) is an experimental radiotherapy technique used to treat the most aggressive types of brain tumors that cannot be surgically removed from the human body. To date, clinical trials of BNCT have been initiated at only a handful of reactors around the world, but advanced studies on BNCT are still being carried out in numerous research centers where the suitable or convertible reactors are available. Construction of BNCT facilities is justified only at some existing reactors. Others can possibly be adapted for BNCT by using fission converters to modify the energy spectrum of the primary neutron beam, which makes it useful for treatment purposes. The BNCT converter, designed for use in the MARIA research reactor at the National Centre for Nuclear Research (NCBJ) in Świerk near Warsaw, Poland, consists of 99 fuel rods (containing low-enriched uranium) inside of the aluminum box. Since its installation affects the core layout and possibly may affect the normal operating regime of the reactor, additional safety analyses must be performed to prove the existence of sufficient safety margins. In this study modern Computational Fluid Dynamics (CFD) techniques have been applied to assess the maximum temperature of the rod wall surfaces, the temperature difference between the inlet and outlet of the converter channel, as well as the maximum and average velocity of the fluid and to compare them with the results presented in the reference analytical study.

Keywords: CFD, Research reactor MARIA, Safety limits, BNCT, Fission converter, Świerk Computing Centre

1. Introduction

Boron-Neutron Capture Therapy (BNCT) is an experimental medical technique to treat glioblastoma multiforme (GBM)—widely viewed as the most common and most aggressively malignant type of brain tumor. In general the therapy is as follows. First, a boron solution is injected into the patient's body. This solution is then attracted by tumor cells,

*Corresponding author

Email addresses: piotr.prusinski@ncbj.gov.pl (Piotr Andrzej Prusiński^{*}), slawek@cyf.gov.pl (Sławomir Potempski), manhaz@cyf.gov.pl (Mieczysław Borysiewicz), Karol.Kowal@ncbj.gov.pl (Karol Kowal), Tomasz.Kwiatkowski@ncbj.gov.pl (Tomasz Kwiatkowski), a.m.prusinski@gmail.com (Andrzej Marcin Prusiński)

which are indicated this way for further treatment. Afterwards the patient's ill tissue is exposed to a collimated beam of fast or at least epithermal neutrons which activate the solution and, in theory, kill the tumor. Until now, clinical trials of BNCT have been initiated at only a few reactors in Europe, the USA and Japan. However, advanced studies on BNCT are being carried out in numerous research centers, where suitable or convertible reactors are available [1–4].

Production of a sufficient dose of epithermal neutrons, with an acceptably low background of high energy neutrons, requires special nuclear reactor features. Consequently, the construction of BNCT facilities is justified only at certain existing reactors. Other reactors can be adapted for BNCT by using fission converters [5], as in the case of the MARIA research reactor at the National Centre for Nuclear Research (NCBJ) in Świerk near Warsaw, Poland [6].

The presented work is focused only on thermal hydraulic aspects of the part of an installation that is going to be immersed in the vessel (or “basket” as it is commonly called) of the MARIA research reactor, namely a fission converter, which will feed neutrons to the rest of the installation. This part can be seen as a box-shaped reactor fuel assembly channel with one measurement probe and 98 fuel rods placed in a hexagonal lattice [7]. The new medical equipment will change the core layout and may possibly influence the normal operating regime of the reactor. In order to prove the existence of sufficient safety margins, an analytical study [7] was carried out by the staff of the MARIA Reactor Operation Division at NCBJ.

However, this study has a number of limitations, e.g. for each of the 98 rods one may expect its own unique heat flux spatial distribution, which makes it problematic to realistically predict the temperature distribution of the rods by analytical calculations. Instead, the analytical calculations of the heat transfer were performed only for one—though the most thermally loaded—rod. For the purpose of analytical study, it was assumed that this rod replaces the probe. In that sense any further calculation accounts for the existence of 99 rods. The reference heat flux generated by this rod was assumed to be more than 2.5 times higher (up to 5 kW) than the one expected

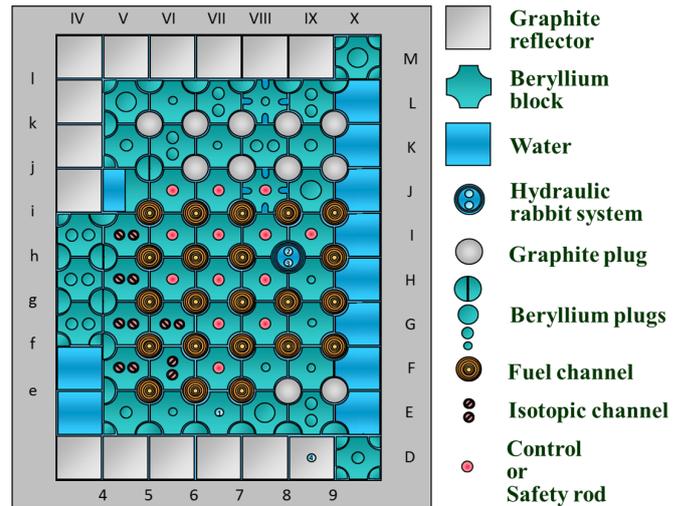


Figure 1: Sample configuration of MARIA's core

from the real case (1.92 kW), because of the conservative approach adopted. However, it still does not account for the thermal effect of all other 98 rods on that one, which is supposed to be an important contributor to the surface temperature of the most thermally loaded rod and to the final temperature distribution in the flow domain of the converter.

The aim of this research is to provide a validation of the analytical computation results of the reactor safety-related margins, by means of an extended (full scale) 3D study accounting for the existence of all 99 rods, before new equipment will be installed. For that purpose modern Computational Fluid Dynamics (CFD) techniques have been used. In this study, parameters of interest were:

- maximum temperature of the rod wall surfaces,
- difference in fluid temperatures between inlet and outlet of the channel,
- maximum and average velocity of the fluid.

The combination of realistic input data supported by uncertainty analysis, that in fact provides a conservative operational margin, with the best estimate codes is a common practice in the nuclear industry.

2. Research reactor MARIA

The research reactor MARIA is a multi-purpose high flux reactor of a pool type, moderated with wa-

ter and beryllium with graphite reflector and pressurized channels consisting of concentric six-tube assemblies of fuel elements. It has been designed with a high degree of application flexibility. The fuel channels are situated in a matrix containing beryllium blocks and enclosed in a lateral reflector made of graphite blocks in aluminum cans (Fig. 1). MARIA is equipped with vertical channels for irradiation of target materials, a rabbit system for short irradiations and seven horizontal neutron beam channels.

MARIA went critical for the first time in December 1974 and remained in operation until 1985 when it was shut down for modernization. The modernization encompassed upgrading and refurbishment of technological systems. In particular, the efficiency of the ventilation and cooling systems was improved. In 1993 the MARIA reactor was put into operation again [8].

The main areas of reactor application are as follows:

- production of radioisotopes,
- testing of fuel and structural materials for nuclear power engineering,
- neutron radiography,
- neutron activation analysis,
- neutron transmutation doping,
- research in neutron physics and condensed matter physics.

The main characteristics and data of MARIA reactor are presented in Table 1.

3. Experimental facility

The facility for BNCT has been designed to be located at the MARIA pool type research reactor, which is equipped with vertical channels for irradiation of target materials and seven horizontal neutron channels marked as H2—H8 (Fig. 2). The fuel channels are situated in a matrix, made of beryllium blocks and enclosed by the graphite reflector. Thus the neutron flux is moderated both by water and beryllium blocks.

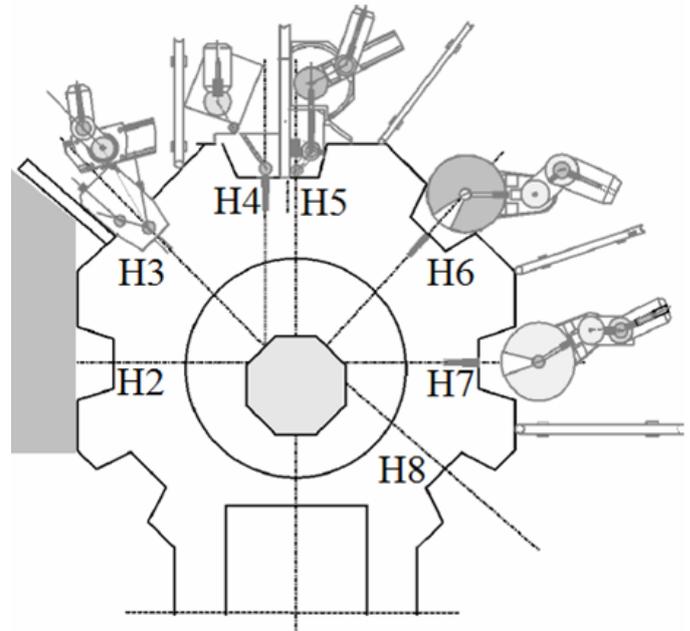


Figure 2: The experimental facilities at the horizontal channels of the MARIA RR [6]

Taking into account all requirements for the place, where the BNCT facility as medical equipment can be located, optimum conditions have been achieved near the mouth of the H2 channel. However, the measurements of the neutron energy spectrum at front of the H2 channel (located near to the reactor core) revealed that the dominating spectrum component is related to the thermal neutrons. Moreover, the calculated total flux density at the mouth of the channel is much lower than measured at the front of it. Thus the flux density of the epithermal neutrons from the MARIA reactor is too low to be directly used for the treatment and for that reason construction of the fission converter at the mouth of the H2 channel is required [6].

The BNCT converter consists of one measurement probe and 98 fuel rods with a height of 0.588 m, containing low-enriched uranium (10% U-235), and is intended to modify the energy spectrum of the primary neutron beam. It is to be located in the graphite matrix instead of one of the reflector blocks at a half-height (Fig. 3). In that configuration thermal neutrons at the mouth of the H2 channel cause the fission reaction in the BNCT converter, which results in the production of fast neutrons. This flux can be then moderated and filtered to obtain an epithermal neu-

Table 1: Research reactor MARIA in numbers

nominal power	30 MW _{th}
reactor type	pool type
water volume:	
- reactor pool	250 m ³
- cooling circuit	20 m ³
moderator	H ₂ O, beryllium
cooling system	channel type
type of fuel channels	pressurized
maximum coolant pressure in:	
- the feeding collector	1.7 MPa
- the draining collector	1.1 MPa*
the nominal flow rate of coolant in the fuel channel	25 m ³ /h (water at 20°C)
fuel element:	
- material	UO ₂ -Al alloy
- enrichment	36%**
- cladding	Aluminum
- shape	6 concentric tubes
- active length	1000 mm
thermal neutron flux density	4.0 · 10 ¹⁴ n/cm ² s
output thermal neutron flux density at horizontal channels	3 – 5 · 10 ⁹ n/cm ² s
maximum wall temperature of the fuel element, accounting for uncertainty factors	180°C

*For calculation purposes 1.2 MPa is taken as a value of a pressure in the fuel channel

**From November 2012, HEU fuel is to be gradually replaced with LEU (19.75%)

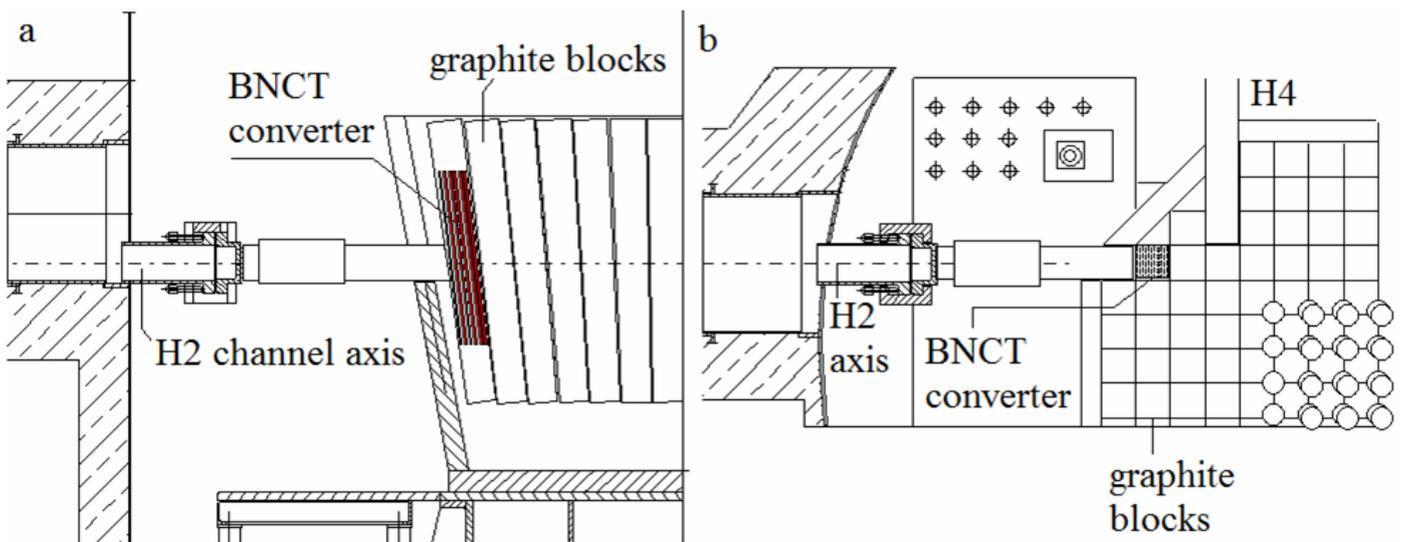


Figure 3: Schematic view of the BNCT line in the MARIA reactor: (a) side view (b) top view [7]

tron beam of the required efficiency, spatial homogeneity and low contamination, which can be used for treatment purposes [6, 7].

Fig. 4 presents the geometrical details of the converter. The converter box is an aluminum thin wall structure—the same as the cladding for the replaced graphite block. The block ends up at the bottom with the holder known as a converter “foot” designed to place it in the right position. Inside of the box there is the converter core fixed on top and bottom by the aluminum separators welded to the box. The converter core itself is a hexagonal rod matrix with a step of 12 mm, as presented in Fig. 4.b. Each rod has a diameter of 10 mm. One of the corner rods (bottom-right corner of the lattice shown in Fig. 4.b.), the closest to the reactor core, has been replaced by a measurement probe to monitor temperature and neutron flux.

4. Analytical study

The reference study underpinning this research is an internal NBCJ document called “Safety Analyses of BNCT converter” [7]. Unfortunately, the documentation is only internal and written in Polish, so unavailable for most readers. Hence, a brief introduction is necessary in order to familiarize the reader with the study.

In general, the safety document sets out the steps taken to ensure that the maximum temperature of the most thermally loaded rod will never exceed 85°C (358 K) for steady state and 136°C (409 K) for transient emergency cases. These steps are as follows:

- making assumptions and sketching a design;
- checking whether the available equipment suits the needs, i.e. if the fuel pins are leakage-tight;
- performing neutron calculations either for MARIA’s core with converter or for the converter only, using either transport or diffusive codes;
- making thermal hydraulic analytical calculation for just one, but the most thermally loaded rod, taking uncertainties into account.

For consistency, the authors would like to underline that the term “analytical study” as used in this paper refers to the thermal hydraulic part of the study.

Going into details, in order to determine the heat generation of the fuel in the BNCT converter, first of all the neutron calculations were performed using transport code WIMS-ANL [9] only for the converter core. It was also assumed that the converter contains 99 fuel rods and the probe was replaced with a rod only to preserve the uniformity of the converter matrix structure. Then, the diffusive code REBUS [10] was applied to determine the results in the framework of the whole core of MARIA (with the converter).

Values obtained this way can be influenced by numerous uncertainties. These uncertainties are caused by calculation uncertainties, variable reactor core configuration and uncertainties coming from the heat transfer model. Hence, the thermal power of the most thermally loaded fuel rod in the converter, adopted in the calculation, was raised to 5 kW instead of taking the 1.92 kW coming directly from WIMS-ANL/REBUS.

The next stage was to perform the calculations of heat exchange in the BNCT converter using the following assumptions:

- only the most thermally loaded rod undergoes analysis,
- calculations are made for the virtual hexagonal channel
- hydraulic diameter assumes the existence of a wetted perimeter calculated on rod surface
- initial conditions are:
 - inlet water temperature: 50°C (323 K),
 - pressure drop across the core matrix: 1400 mm H₂O,
 - height of the rod with the sleeves of separators: 0.59 m,
 - thermal power of cooled rod: 5 kW,
 - extrapolated height of fuel: 0.65 and 1.15 m.

The axial distribution of power density in the most thermally loaded fuel rod will correspond more to the extrapolated height of 1.15 m, which is characteristic for the MARIA reactor core. Therefore, the

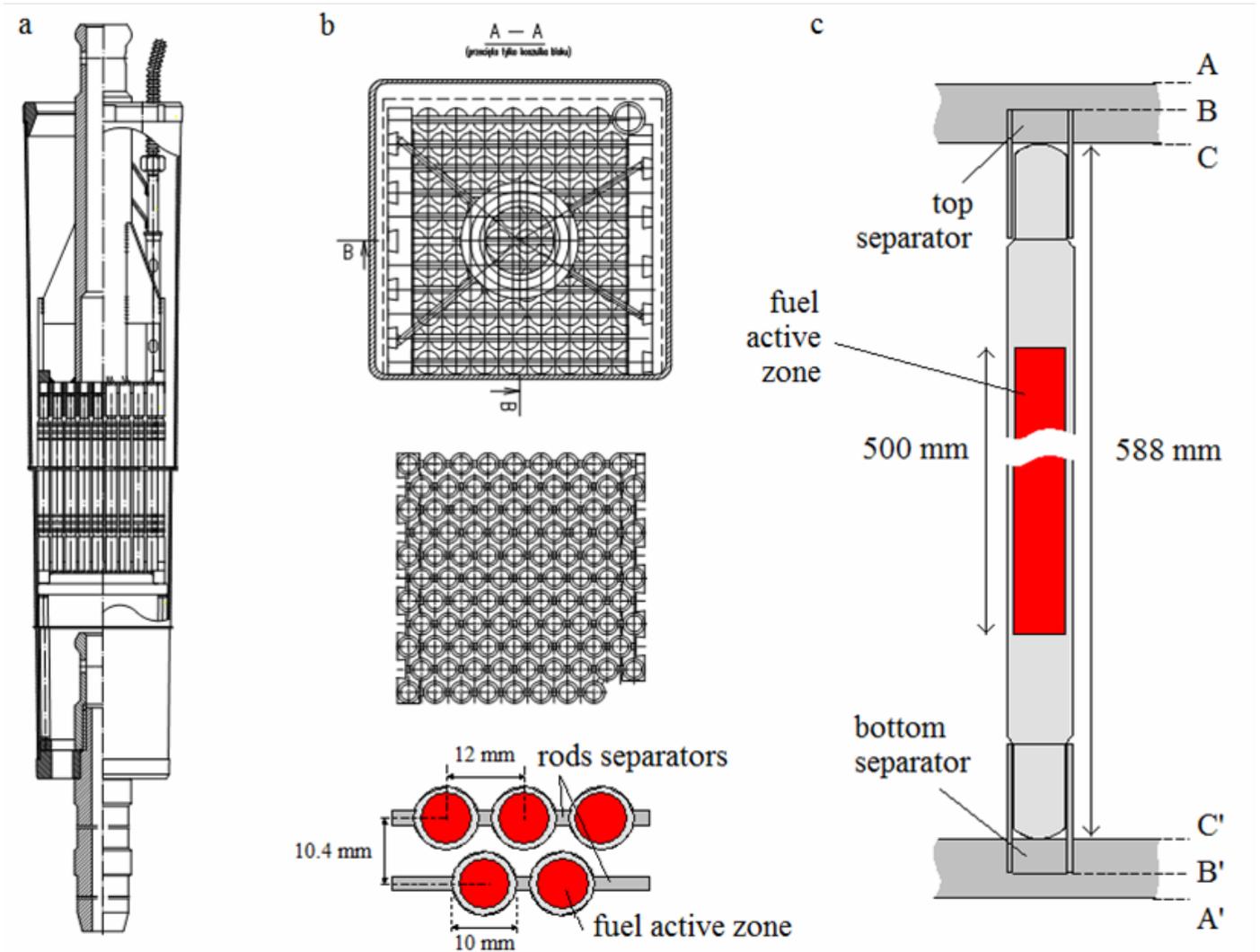


Figure 4: Details of the BNCT converter geometry (column a) side cross-section view of converter box with internals (b) top cross-section view and magnified details (c) the fuel rod installation [7]

wall temperature of that element will reach a maximum near the bottom edge of the fuel and will not exceed 85°C (358 K) for steady state.

5. CFD simulation setup

5.1. Mesh

Due to the high complexity of the geometry, some general assumptions were taken into account when preparing the input CFD geometry and for the further mesh generation process.

The very first geometry used in this study was kept as simple as possible. First of all, instead of the real quadrilateral frustum shape of the channel, a regular cuboid box with dimensions of 118×120×700 mm was used. Although the 99 rod lattice was preserved, the simplifications were used in terms of other channel internals. The simplified geometry used in this study does not consist of channel handlers, internal orifices, i.e. rod spacers etc. In general this geometry can be seen as a box-shaped reactor fuel assembly channel with 99 fuel rods in a hexagonal lattice.

The length of the fuel rods was reduced to just 500 mm, which corresponds to the real active zone height of the fuel. In this case rods are vertical and parallel to all the walls and the flow direction; however, in fact either the channel is rotated about 9° from the vertical axis or the rods are aligned to just one of the walls.

For the purpose of CFD simulation a volume mesh made of about 700 000 tetrahedral cells was generated with the help of the GAMBIT v.2.4.6 program (Fig. 5). The mesh contains over 1.5% highly skewed cells. These cells often exhibit a deterioration of the computational results or lead to numerical instabilities. The other issue is the relative size of cells in the domain, which may also pose a problem to the numerical scheme. There are two approaches overcoming those issues. The first is to use a mixed mesh with different shapes of cells in the same domain. This is a compromise between the number of cells and the recreation accuracy level of the geometry. The other approach is to maximize the number of cells, reducing the difference in cell size so as to achieve a uniform mesh. Due to initial computing limitations, the first approach, with a tetra-hybrid volume meshing method, was chosen for further studies.

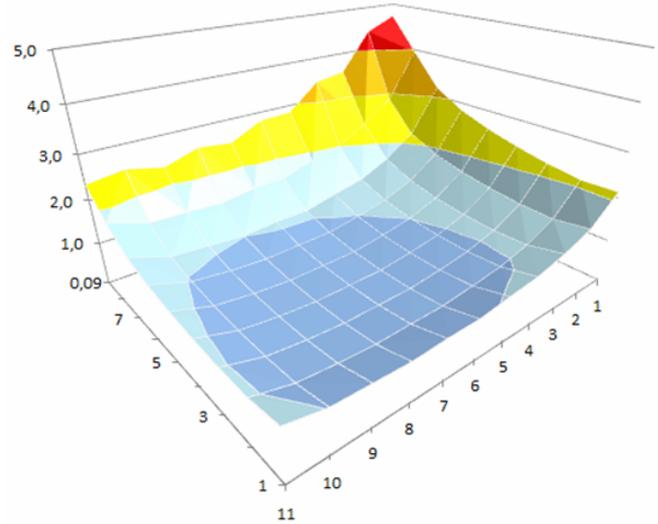


Figure 6: The power distribution over BNCT core lattice [kW]

The use of tetrahedra enables better reproduction of non-orthogonal shapes, i.e. oval, in the flow domain. This is important with regard to the smoothness of their surfaces. This, in turn, means application of the Finite Volume Method (FVM), which is usually better than the Finite Difference Method (FDM), but it demands extra computational effort.

For all the reasons mentioned above, this mesh should be treated as a very rough approximation and should be improved afterwards.

5.2. Solver

For the purpose of the simulations, steady state with the realizable $k-\varepsilon$ turbulence model was applied due to the expected Reynolds number in the range of $Re \sim 10^4$, which implies the existence of turbulent flow. Since the fluid is incompressible and its velocity is relatively low, the pressure-based approach was applied. In this approach, the pressure field is extracted by solving a pressure or pressure correction equation, which is obtained by manipulating continuity and momentum equations.

The ANSYS Fluent platform provides four segregated algorithms for solving Pressure-Based Navier-Stokes (PBNS) equations. These are SIMPLE, SIM- PLEC, PISO and FSM. However, in general, the use of SIMPLE or SIM- PLEC algorithms is recommended for steady-state calculations. Moreover, experiments done in this research have shown no dif-

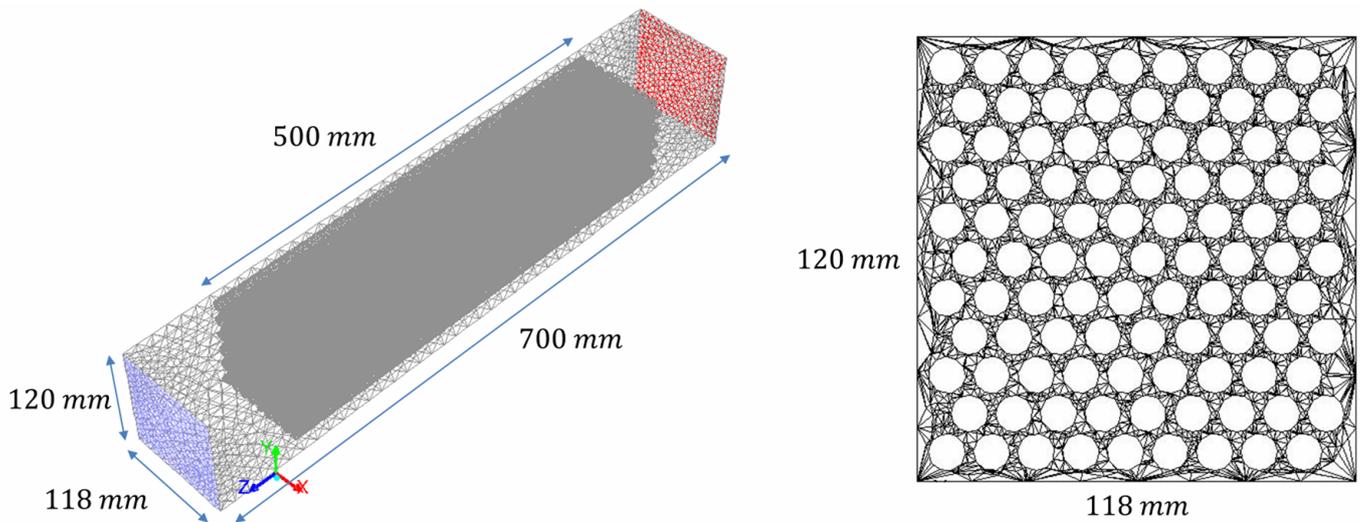


Figure 5: Mesh made of 696 685 cells

Table 2: Initial and boundary conditions

Condition	Definition
Inlet	velocity inlet velocity 1.27 m/s; temperature 323 K
Outlet	outflow
Walls (box)	wall material: aluminum density 2719 kg/m ³ , specific heat 871 J/(kg·K), thermal conductivity 202.4 W/(m·K) stationary wall; no slip condition; roughness constant 0.5; roughness height 0 m (smooth walls) thermal conditions: heat flux according to Fig. 6
Fluid zone	water liquid density (constant) 998.2 kg/m ³ , dynamic viscosity 0.001003 Pa·s, specific heat 4182 J/(kg·K), thermal conductivity 0.6 W/(m·K), gravity -9.81 m/s ² (z-axis)
Operating conditions	operating (Boussinesq) temperature 323 K

Table 3: Numerical model

Option	Definition
Solver type	Pressure-Based
Velocity formulation	Absolute
Time	Steady
Model	Energy: On Viscous model: realizable k - ϵ , Near-Wall Treatment: Standard Wall Functions with option: Viscous Heating
Pressure-Velocity coupling	Scheme (segregated): SIMPLE
Spatial discretization	Gradient: Green-Gauss Cell Based, Pressure: Standard, Momentum: First Order Upwind, Turbulent Kinetic Energy: First Order Upwind, Turbulent Dissipation Rate: First Order Upwind, Energy: First Order Upwind

ference between the results obtained using SIMPLE and SIMPLEC (Table 3).

6. Results and comments

6.1. Results

The preliminary results of CFD simulations, as depicted by Figs. 7 and 8, performed for steady state conditions are as expected. Temperature profiles are impacted by introducing 98 new rods and keeping the flow regime at about the same Re number level as in the analytical study. In Table 4 one can find a comparison between the analytical study and results obtained from simulations.

Although the results are comparable, i.e. velocities, the most disturbing is the maximum wall surface temperature (Fig. 7) coming from the CFD simulation, which is 20 K higher here than the one from the analytical calculation and at the same time the temperature difference between inlet and outlet is 3 times lower.

However, higher temperature is not just an effect of adding extra rods. It is also due to the converter core lattice configuration or, to be more specific, due to the 6 mm relative shift between the odd and even rods rows. This shift plays a major factor in the flow pattern, by creating possibilities for flow bypass at the end of the rows, disturbing velocities and in turn

heat distribution, which was not accounted for in the analytical assumptions but exists in the real model, which is ready to be used in the reactor. The analytical study provides the data for velocity in the core region of the channel. It is 2.82 m/s, which matches the results from the CFD experiment. However, the flow pattern is shown by the simulation to be more complicated and, as mentioned earlier, in the case of velocities a relatively large difference is evident between the inner and outer space of the core (Fig. 9). While the fluid passing through the inner-core space flows at an average speed of 2 m/s, the velocity of the rest rises to even 3.7 m/s. It is surmised that this difference comes from the size of the gap space between the rods and the channel walls, which varies from 3 to 9 mm (the essence of the 6 mm shift between the rods and the channel walls, which varies from 3 to 9 mm (the essence of the 6 mm shift problem mentioned above), especially when compared to the constant 2 mm distance between the rods. The velocity in the outer-core (and indirectly inner-core) region is in this sense a function of the gap thickness. The bigger the gap, the faster the flow is in the outer space and in turn the slower it is in the inner-core region. Slowing the flow in the inner space, where there is a relatively small amount of coolant with limited heat capacity surrounding the high energy rods, causes impaired heat transfer and this leads finally to

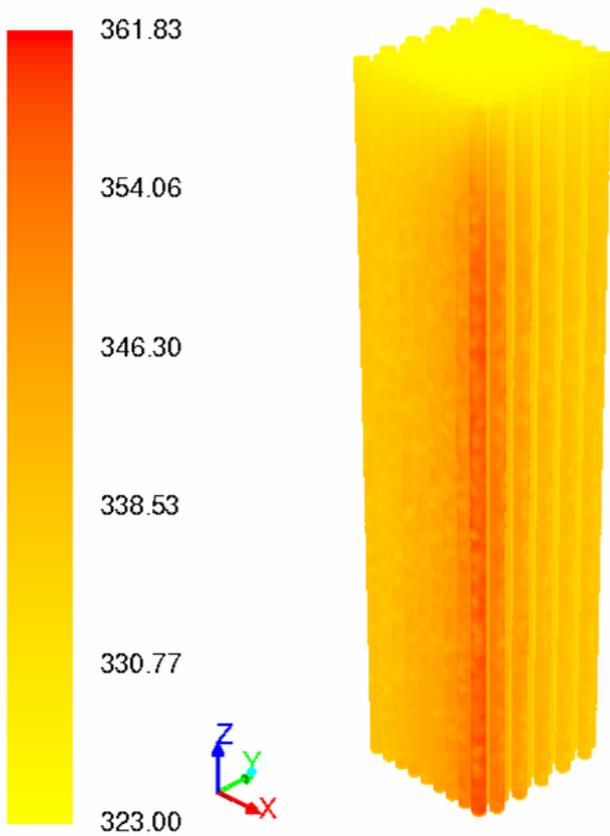


Figure 7: Rod temperatures (K)

quite large discrepancies between the maximum temperature of the rod surface obtained from the simulation of the real case and from the analytical study. This should be taken into account in any further studies.

Fig. 7 and Fig. 8 also present the non-uniform spatial temperature distribution which is directly related to the unique heat distribution of the converter rods (see Fig. 6). It needs to be borne in mind that each rod has its own power. This effect comes from the fact that the converter core is activated by neutrons arriving from MARIA's core and as the most thermally loaded rod (bottom-right corner on Fig. 8) is the closest one to MARIA's core, so it is the rod most vulnerable to neutron bombardment.

Finally, one can claim that the presented results cannot constitute a basis for formulating such conclusions due to the low quality of the mesh. While one has to take into account the fact that the results are preliminary and of low resolution, they are still in good agreement with the physics and above all con-

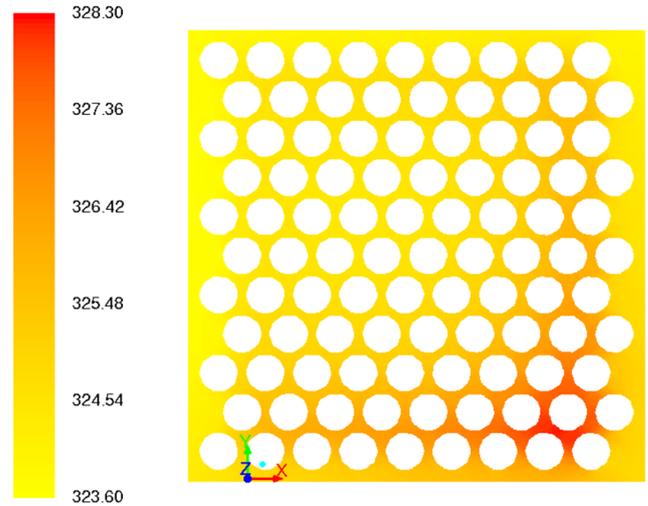


Figure 8: Fluid temperature distribution at the bottom end cross-section of the rods zone (K) the hottest rod located in the bottom-right corner

verged at a sufficient level of residuals (Fig. 10).

6.2. 6.2. Computational performance

A precise determination of the safety margins of the reactor core after a change of configuration was prepared using ANSYS Fluent v.13/14 software. The calculations were performed at the Interdisciplinary Centre for Mathematical and Computational Modelling (ICM Warsaw) on halo2 cluster, whose nodes consist of 16 cores—4 AMD Quad-Core Opteron 835X processors for each. In addition, the results of these calculations were used to set guidelines for further efficient simulations. During the works, some benchmarks were made and their results are presented in this paper.

The calculations were performed for the geometry set out above, in a domain consisting of 696,685 tetrahedral elements. The number of iterative steps was 1,500 on each occasion while the core number varied from 1 to 128. Table 5 below shows the average, minimum and maximum computation time obtained from 10 trials against a different number of cores.

The average computational time decreases from 433.6 to 8.9 min with the core number ranging from 1 to 64. However, as the number of cores increases above 64 the speedup flattens, as illustrated in the figures below (Fig. 11 and Fig. 12).

Table 4: Analytical vs. evaluated results

Parameter	Analytical	Evaluated
V_{ave} in channel, m/s	2.82	2.0–3.7
T_{max} of the rod surface, K (H=65 cm)	341.80	361.83
ΔT between inlet and outlet, K	9.30	0.9–3.5
Heat transfer coeff, α_{hrod} , W/m ² K (*)	31.2E+03	8–20E+03
Hydraulic diameter, mm (**)	5.90	7.12
Reynolds number	3.21E+04	2.02E+04
Flow area cross-section/rod, mm ² (**)	46.26	63.85

*Along the rod

**The difference in dimensions in the case of flow area and in turn hydraulic diameter comes from the technical limitations of the 99 rods model, where the channel cannot be narrower than 112×114 mm. Thus the smallest flow area per rod of 50.43 mm² is possible

In addition, there is a much lower than expected speedup of calculations with the increase in the number of cores from 16 to 32 (Fig. 12). On the other hand, the speedup obtained for 64 cores is quite high (7.5 times faster) in comparison to the value for 32. This is a remarkable result and one that was proven by ten trials, which means it is not a random fluctuation but an obvious trend. For now there is no clear explanation, but the reason is probably related to the architecture of the cluster, since every case was performed with the same domain, algorithm and computational scheme. The only thing that changes here

Table 5: Computation time against number of cores

cores num./ time, min	1	16	32	64	128
average	433.6	91.6	67.5	8.9	9.6
minimum	424	84	50	8	8
maximum	460	113	85	14	12

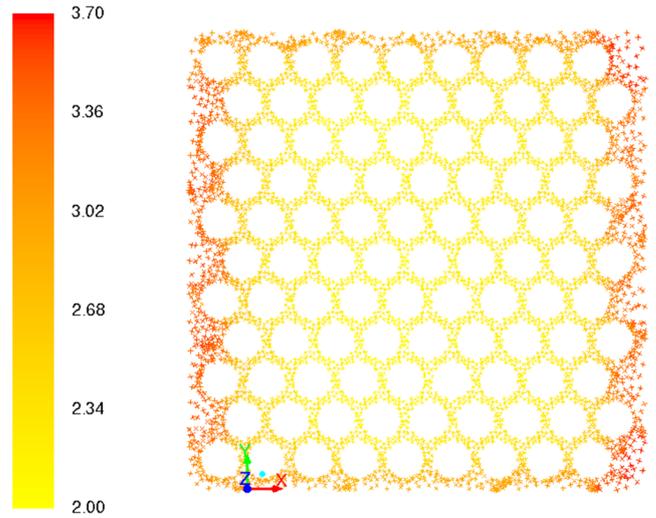


Figure 9: The velocity vectors at the bottom end of the rods (m/s)

is the number of cluster nodes.

As is shown in Fig. 11 and Fig. 12 the configuration of 64 cores seems to be the most suitable for this domain when using halo2 architecture.

In general, the simulation time optimization is an important standard procedure adopted in other studies of the authors. However, it is done only for informational purposes, to give users some indication of what choice will be better from the practical point of view without focusing on the true cause of the problem, which in this case seems to be the computing facility. This way the authors build a database of good practices.

The presented data should be treated in the same way, simply informational. They are not crucial for the article itself.

7. Further development

The project should be viewed as an intermediate step in the larger research process as it will be carried out in future, utilizing access to a new computing cluster. Nevertheless some further developments are required before the final stage is achieved. This means, first of all, building a new improved mesh that accounts for the possibility of real near-wall modeling instead of the standard wall function approach. At present, trials are in progress with a new 8 million

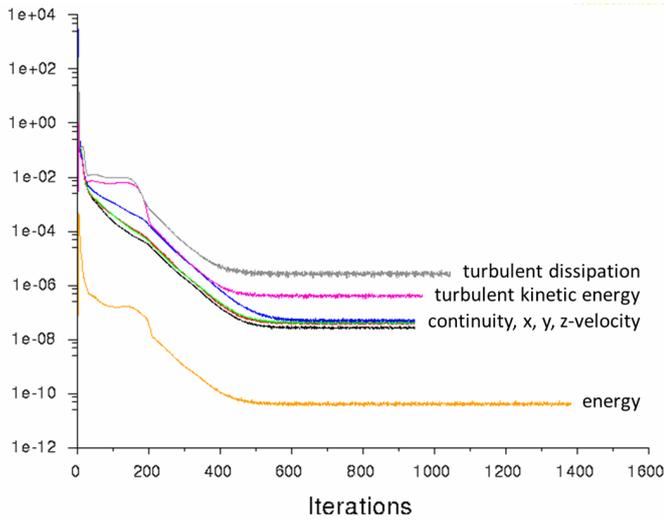


Figure 10: The simulation residuals

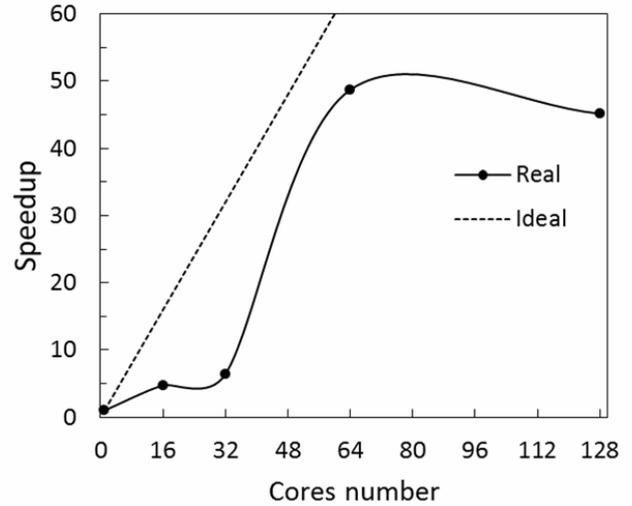


Figure 12: Real and ideal speedup

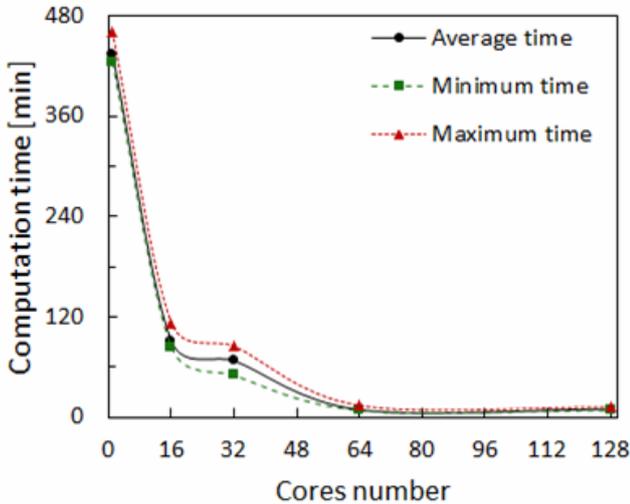


Figure 11: Computation time against the number of cores

cell mesh, consisting of surface layers dedicated to the boundary layer parameters tracking (Fig. 13).

Although the wall function approach was designed with high Reynolds number flows and should be valid for this case, it should be borne in mind that the converter is a kind of heat exchanger with relatively huge exchange areas in the form of rods, which do not leave much space for the coolant. In fact it can be assumed that the experiment deals with the flow almost entirely in the boundary layers. The problem is that the wall function approach does not resolve the viscosity-affected region; instead it is “bridged” by the wall functions. In contrast, near wall model-

ing resolves the near-wall region all the way down to the wall and the turbulence models ought to be valid throughout the near-wall region, resulting in a better heat transfer model.

When the new mesh—or the geometry in general—is considered, its dimensions should be determined afresh. In the case of X and Y direction it should be checked how the gap between the rods and the channel walls influences the velocities and temperature distribution. With the Z direction, the outlet space should be longer so as to obtain the parameters for fully mixed coolant, which is not possible with the current mesh.

Some improvements should also be made from the numerical point of view. To date, the First Order Upwind scheme was used for fast processing. However, for more robust results use it will shortly involve QUICK and Third-Order MUSCL schemes.

Another simplification was to apply a realizable $k-\varepsilon$ turbulence model. According to the ANSYS Fluent Theory Guide [11], the term “realizable” means that the model satisfies certain mathematical constraints on the Reynolds stresses, consistent with the physics of turbulent flows. Nevertheless, no-one has yet checked its full applicability to the model and further uncertainty studies in this topic are already scheduled.

Finally, in order to prove the accuracy of the simulation results, they have to be validated against ex-

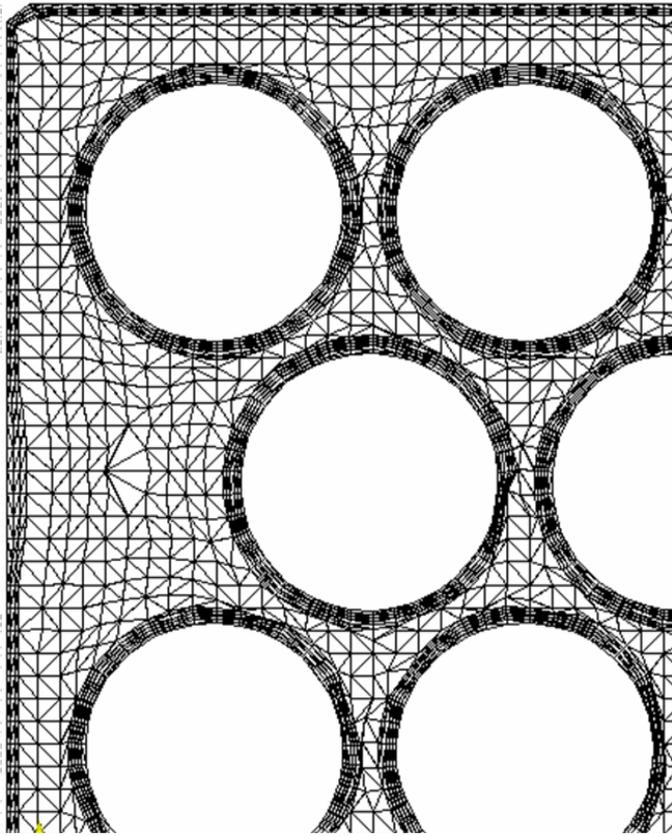


Figure 13: New mesh containing boundary layers cells

periment in the reactor, but since the latter has been delayed, other steps are being considered. As was mentioned, this project is under development with the use of ANSYS Fluent v.13/14 from the very beginning. However, other CFD codes, i.e. OpenFOAM and Trio_U, are taken into account and will be used to validate the results. The same concerns the CATHARE [12]—System Thermal Hydraulic (System TH) code. Although CATHARE is unable to provide an exact value of, for example, maximum rod wall surface temperature, because it is intended to model full-circuit-scale problems rather than component scale issues, it is helpful for a general perspective on physics or the correctness of applied boundary conditions.

The other issue at play is that the nuclear industry relies mostly (if not solely) on System TH codes, which are considered to be the best solution for a low price in a short time. This short time comes in fact from the limitation of System TH codes, which implies a bigger scale of elements in the same domain as in CFD and in turn lower resolution, but instead it

offers lower computational effort.

Validation by means of using a different class of codes is also a common practice in nuclear design. These codes can be applied either separately or coupled. The latter option has become popular recently. It is interesting to use both of them at once, assuming different scales of the problem in the same experiment.

The use of several different codes will assure an appropriate level of confidence. It will also broaden the range of specialists able to share their experience and contribute to further studies.

Although the project is still at an early stage, the research done thus far has thrown up some new issues that were not previously taken into account, i.e. the influence of all 99 fuel rods on the flow domain. This means that the use of CFD techniques for reactor safety studies are of value and their application looks set to become a required element of safety analysis in the future.

Acknowledgments

The authors of this paper wish to thank the staff of Reactor MARIA Operation Division at NCBJ, especially Krzysztof Pytel and Władysław Mieszczenko for their help and support.

The work was supported by the EU and MSHE grant no. POIG.02.03.00-00-013/09

References

- [1] R. F. Barth, J. A. Coderre, M. G. H. Vicente, T. E. Blue, Boron neutron capture therapy of cancer: Current status and future prospects, *Clinical Cancer Research* 11 (11) (2005) 3987–4002. doi:10.1158/1078-0432.CCR-05-0035.
- [2] Y. Nakagawa, K. Pooh, T. Kobayashi, T. Kageji, S. Uyama, A. Matsumura, H. Kumada, Clinical review of the Japanese experience with boron neutron capture therapy and a proposed strategy using epithermal neutron beams, *Journal of Neuro-Oncology* 62 (2003) 87–99. doi:10.1023/A:1023234902479.
- [3] A. Z. Diaz, Assessment of the results from the phase i/ii boron neutron capture therapy trials at the Brookhaven National Laboratory from a clinician's point of view, *Journal of Neuro-Oncology* 62 (2003) 101–109. doi:10.1007/BF02699937.
URL <http://dx.doi.org/10.1007/BF02699937>

- [4] J. Capala, B. H.-Stenstam, K. Sköld, P. afC. Persson, E. Wallin, A. Brun, L. Franzen, J. Carlsson, L. Salford, C. Ceberg, B. Persson, L. Pellettieri, R. Henriksen, Boron neutron capture therapy for glioblastoma multiforme: clinical studies in sweden, *Journal of Neuro-Oncology* 62 (2003) 135–144. doi:10.1007/BF02699940. URL <http://dx.doi.org/10.1007/BF02699940>
- [5] O. Harling, K. Riley, Fission reactor neutron sources for neutron capture therapy — a critical review, *Journal of Neuro-Oncology* 62 (2003) 7–17. doi:10.1007/BF02699930. URL <http://dx.doi.org/10.1007/BF02699930>
- [6] N. Golnik, K. Pytel, Irradiation facilities for bnct at research reactor maria in poland, *Polish Journal of Medical Physics and Eng.* 12 (3) (2006) 143–153.
- [7] K. Pytel, W. Mieleszczenko, M. Dorosz, T. Kulikowska, Z. Marcinkowska, Safety analyses of bnct converter, Internal report, NCBJ (2010).
- [8] G. Krzysztozek, A. Gołąb, J. Jaroszewicz, Operation of the maria research reactor, Annual report, IEA POLATOM (2010).
- [9] J. Deen, W. Woodruff, C. Costescu, L. Leopando, WIMS-ANL User Manual, Rev. 6, ANL/TD/TM-99-07 (2004).
- [10] A. Olson, A User's Guide for the REBUS-PC Code, Version 1.4, ANL/RETR/TM-32 (2011).
- [11] ANSYS Inc., ANSYS Fluent Theory Guide, Release 14.0 (2011).
- [12] Lavalie G. et al.: CATHARE 2 v2.5 2: Description of the Base Revision 6.1 Physical Laws Used in the 1d, 0d and 3d Modules (2008).
- [13] J. Ferziger, M. Perić, Computational Methods for Fluid Dynamics, 3rd Edition, Springer, 2002.
- [14] J. Tu, G. Yeoh, C. Liu, Computational Fluid Dynamics: A Practical Approach, Elsevier Inc., 2008.
- [15] H. Versteeg, W. Malalasekera, An Introduction to Computational Fluid Dynamics The Finite Volume Method, Prentice Hall, 2007.