

CFD analysis of the effect of a fuel assembly blockage in a liquid metal cooled fission reactor

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CFD ANALYSIS OF THE EFFECTS OF A FUEL ASSEMBLY
BLOCKAGE IN A LIQUID METAL COOLED FISSION
REACTOR



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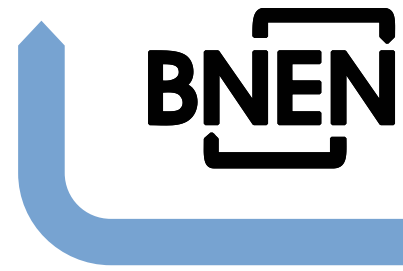
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Master of Science in Nuclear Engineering



Thesis Summary Page

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Title:

CFD Analysis of the Effects of a Fuel Assembly Blockage in a Liquid Metal Cooled Fission Reactor

Abstract:

The Belgian nuclear research centre SCK•CEN located in Mol endeavours to develop the new generation reactor MYRRHA. The characteristics that differentiate this technology are the lead-bismuth-eutectic coolant and spallation target, which sustains the fission chain reaction, being it a subcritical reactor. To ensure the safety of this complicated project, some postulated accidental conditions must be taken into account, in order to ensure its safe operation and reduce the probability of such accidents with the appropriate design.

In the present work the fluid behaviour in presence of a local internal blockage in a wire wrapped fuel assembly will be studied. Indeed, through CFD simulations, the hydraulic as well as the thermal fields in presence of both solid and porous blockage are analysed, to tackle the fuel assembly safety aspects. Additionally, the case scenario with heat-emitting porous blockage has been investigated as well. Particular attention has been given to the process to define the most appropriate mesh for the domain, both on the meshing algorithm itself and on the level of refinement desired to obtain meaningful results. Similar treatment has been applied to the solving modelling method decision. In addition, a detailed sensitivity analysis on the influence of different parameters on the temperature distribution within the fuel bundle has been done, in order to understand the difference between the numerical results and the experimental data. In conclusion, due to the heterogeneous formation origin of such blockages, a parametric study on the impact of blockage properties, i.e. porosity and self-heating, on the thermohydraulic flow field has been performed.

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Summary

The Belgian nuclear research centre SCK•CEN located in Mol endeavours to develop the new generation reactor MYRRHA. The characteristics that differentiate this technology are the lead-bismuth-eutectic coolant and spallation target, which sustains the fission chain reaction, being it a subcritical reactor. To ensure the safety of this complicated project, some postulated accidental conditions must be taken into account, in order to ensure its safe operation and reduce the probability of such accidents with the appropriate design.

In the present work the fluid behaviour in presence of a local internal blockage in a 19-pin wire-wrapped rod bundle representing the MYRRHA fuel assembly is studied. Indeed, through numerical CFD simulations, the hydraulic as well as the thermal fields in presence of both solid and porous blockage are analysed, to tackle fuel assembly safety aspects. Firstly, a single solid blockage occupying one single subchannel is modelled, in order to approach the validation of the code through the comparison with the experimental data performed in the KIT-KALLA tests, within the European project MAXSIMA. Particular attention has been given to the process to define the most appropriate mesh for the domain, both on the meshing algorithm itself and on the level of refinement desired to obtain meaningful results. Similar treatment has been applied to the solving modelling method decision. In spite of this, the results of these numerical assessments are exhibiting big differences in the prediction of temperatures at the thermocouple positions present in the test facility, as it has been described in the numerical simulations done by the partner institution NRG.

For this reason, a detailed sensitivity analysis on the influence of different parameters on the temperature distribution within the fuel bundle has been done, in order to understand the difference between the numerical results and the experimental data. Specifically, the influence of buoyancy, thermocouple position, turbulence model, mesh refinement has been evaluated and all these studies show little sensitivity. Only the inclusion of conduction in the electrical heater has showed a higher impact by decreasing the blockage temperatures.

In the second place, both the case scenarios with non- and heat-emitting porous blockage has been investigated as well. As far as the first aspect is concerned, results obtained show that compared to a solid blockage, the implemented degree of porosity leads to lower temperatures at the cladding surface where the TCs are embedded, since even if limited, the flow of coolant is allowed to a certain extent. Porous blockages with self-heating present an opposite trend: the effect of the

internally generated power is clearly the substantial increase in the temperatures in the blocked region.

In conclusion, due to the heterogeneous formation origin of such blockages, a parametric study on the impact of blockage properties, i.e. porosity and self-heating, on the thermohydraulic flow field has been performed. Given the simulations performed, it has been possible to conclude that, although the overall behaviour observed is common for all cases simulated with the different porosities, the maximum temperatures are affected only marginally by the change in this parameter. Contrarily, the impact of the change in the generated power level shows that overall behaviour of the temperature profiles is enhanced with increasing power, and the maximum temperature steadily increase while going to full power conditions.

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Glossary

ADS	A ccelerator D riven S ystem	MA	M inor A ctinides
Avg	A verage	MAXSIMA	M ethodology, A nalysis and eX periments for the " S afety I n MYRRHA A ssessment
BU	B urn U p		
CFD	C omputational F luid D ynamics	ML	M easuring L evel
DiD	D efence-in- D epth	MOX	M ixed O xide (U, Pu)O ₂
FANC	F ederal A gency for Nuclear C ontrol	MYRRHA	M ulti-purpose h Y brid R esearch R eactor for H igh- tech A pplications
FP	F ission P roduct	NRC	N ational R egulatory C ommission
Gen IV	G eneration I V		
GHG	G reen- H ouse G as	PDE	P artial D ifferential E quation
IAEA	I nternational A tomie E nergy A gency	R&D	R esearch & D evelopment
KIT	K arlsruhe I nstitute of T echnology	RES	R enewable E nergy S ources
KALLA	K arlsruhe L iquid M etal L aboratory	RMS	R eynolds S tress M odel
LBE	L ead- B ismuth- E utectic	SCK•CEN	S tudieCentrum voor K ernenergie • C entre d'Étude de l'énergie N ucléaire
LFR	L ead F ast R eactor		
LINAC	L Inear A ccelerator	TC	T hermo C ouple
LMFBR	L iquid M etal F ast B reeder R eactor	UO ₂	U ranium D i O xide
LWR	L ight W ater R eactor	WENRA	W estern E uropean N uclear R egulators' A ssociation

Chapter 1 – Introduction

1.1 Nuclear power and climate change

In the present days, climate change, CO₂ emissions, clean energy production, total electrification are just some of the most abused words that accompany the world's population in daily life. It is nevertheless true that those are problems that have to be tackled quickly and effectively in this transitional period where a continuously increasing demand of energy is limited by issues linked to global warming, such as phasing-out from fossil energy sources, limitation in GHG emissions and still limited technological development and efficiency in clean energy production. It is straightforward that in order to comply with the downsides of climate change, it is necessary to reduce the emission of polluting gases, and the more efficient way to do it is by gradually dispose of the use of fossils fuels by the end of the century. Nevertheless, this ambition cannot be reached unless all available low carbon energy sources are implemented. Besides, only conventional renewable energy sources (RES) are not sufficient to achieve this task.

In specific, in order to limit the global temperature increase to 1.5°C above pre-industrial levels, which is necessary to avoid catastrophic consequences to the environment and population as stated in the Paris Agreement, 90% of the electricity in 2050 has to come from low carbon options [1].

Although the public's mistrust in nuclear power is challenging every future sustainable action regarding electricity production, nuclear power, along with other more developed and exploited RES, produces very low GHG emissions per unit of electricity generated in its life cycle, as visible in Figure 1. It is visible that this is true even when the whole life cycle, i.e. from mining to decommissioning and waste management, is accounted.

The other advantages of involving nuclear power as part of an integrated low carbon solution to address climate change are that it can provide a continuous reliable low carbon power, it responds to the variation in the daily electricity load and it compensates the demand within the frequency regulation, ensuring a stable energy system. These aspects allow nuclear power to support a higher deployment of variable RES, which have currently a fossil fuel generation as backup capacity, due to their economic efficiency and reliability which restricts their utilization to just a fraction of the energy power needs [2].

On the other hand, despite nuclear power plants do not generate almost any CO₂, all the related radioactive waste products are a dangerous burden to deal with, even for the future generations.

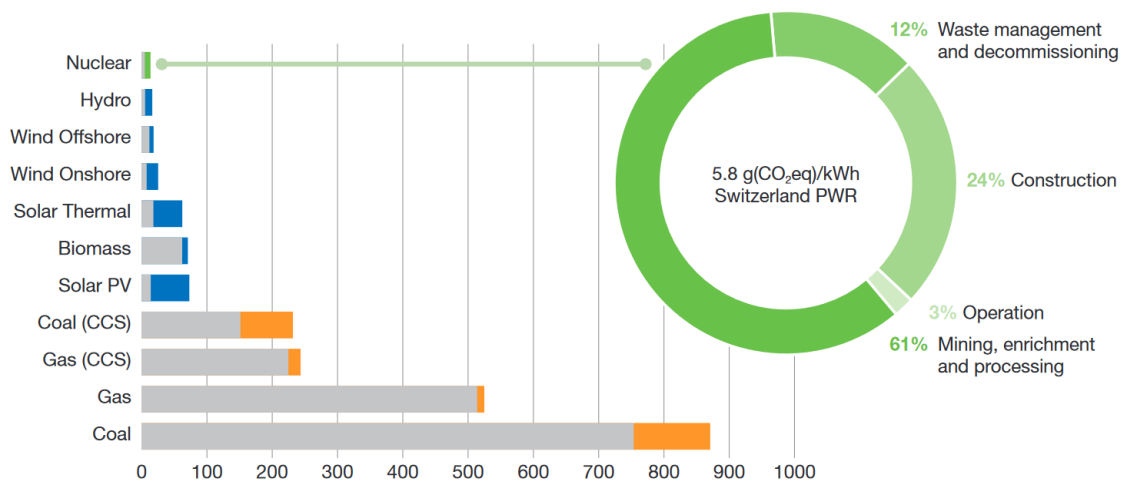


Figure 1 – Life cycle GHG emissions per kWh (gCO₂-equivalent/kWh) [1]

As Robert Spaemann states, it is a present responsibility to pass on the basic conditions of wellbeing undiminished, since society has not the right to deprive the future generation of the natural resources that it have inherited [3].

Nevertheless, management solutions exist for all types of waste arising from nuclear power operations and a vast potential for a broader development of its technologies is foreseen on the longer term, to favour nuclear energy's role as a valuable alternative to fossils fuel deployment and a stable complement to the other sustainable sources of energy, according to what is stated in the nuclear energy technology roadmap [4].

Among all the new strategies that are under advancement in order to reach a more energetically sustainable future, innovation in the field of nuclear reactor technology and improvements in development of new solutions for the treatment of radioactive waste have been considered as the most effective ones. Within this framework, different options have been identified to achieve the above-mentioned goals and as far as safety and radioactive waste dealing are concerned, fast spectrum nuclear reactors and accelerator driven systems (ADS) are currently the most promising ones.

1.2 Generation IV Reactors and Accelerator Driven Systems

As it has been already explained in the previous section, one of the major concerns related to nuclear power production is the generation of high-level nuclear waste by fission reactions. Figure 2 clearly depicts what occurs in the currently operating LWR: a neutron hitting the slightly enriched uranium fuel, composed by the fissile isotope U-235 and the fertile U-238, causes its fission into two smaller and lighter nuclei, i.e. fission products (FP), and the generation of an

average of 2.5 new neutrons per fission reaction, which in turn will produce other fission reactions. Nevertheless, a neutron can be captured by the U-238 to create a long sequence of other fission products through transmutation² and radioactive decay.

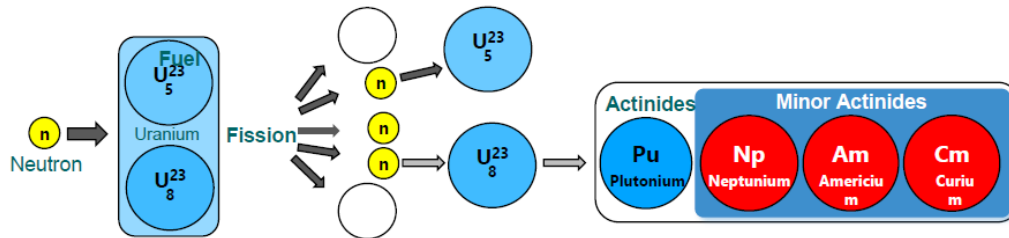


Figure 2 – Fission reaction [42]

Table 1 further analyses the content of 1 ton of spent nuclear fuel retrieved at its end of cycle at a level of BU around 50 GWd/ton [6]: it is relevant to underline that uranium and plutonium could be recycled into MOX fuel through the already established reprocessing³ processes and reused then as new fresh fuel. Nowadays, the preferred option is to store the FP into the deep geological disposal, where they will be contained and permanently isolated [7]. Among these the long-lived MA, principally Neptunium, Americium and Curium, are characterized by a high radiotoxicity and heat emission. It is straightforward that the hazard related to these elements must be taken into account, and therefore the necessity of transmutation, which advantage is depicted in Figure 3, in order to reduce the most noxious component of the radioactive waste [8]. The spent nuclear fuel once retrieved at its end of cycle from current water-cooled reactors is characterised by an increase in radiotoxicity by a factor 10^3 relative to the value of natural uranium ore.

Content	Element
935 kg	U
12 kg	Pu
~2.5 kg	MA
1 kg	Np
0.8 kg	Am
0.6 kg	Cm
~50.5 kg	FP

Table 1 – Mass content of 1 ton of spent nuclear fuel [6]

² Transmutation converts radioactive substances with a long-life span into less toxic substances with a short life span, through neutron capture of these radioactive products generated by fission. [5]

³ Nuclear reprocessing is the chemical process by which the unused uranium and plutonium are separated from the other elements in the spent nuclear fuel retrieved from the nuclear power plants, and that can be then reused in new cycles.

This will decrease to the background level in more than 300 millennia if no actions on the radioactive waste are taken, that is open cycle with direct disposal in the geological depository. If fuel reprocessing is implemented, i.e. separation and recycling only of the uranium and plutonium content, the time span necessary to reach natural radiotoxicity can be lowered already by 30 times, however the striking improvement is achieved through transmutation, where the final volume of residual waste is reduced by a factor 100 and the natural radiation level is already reached after 300 years [9].

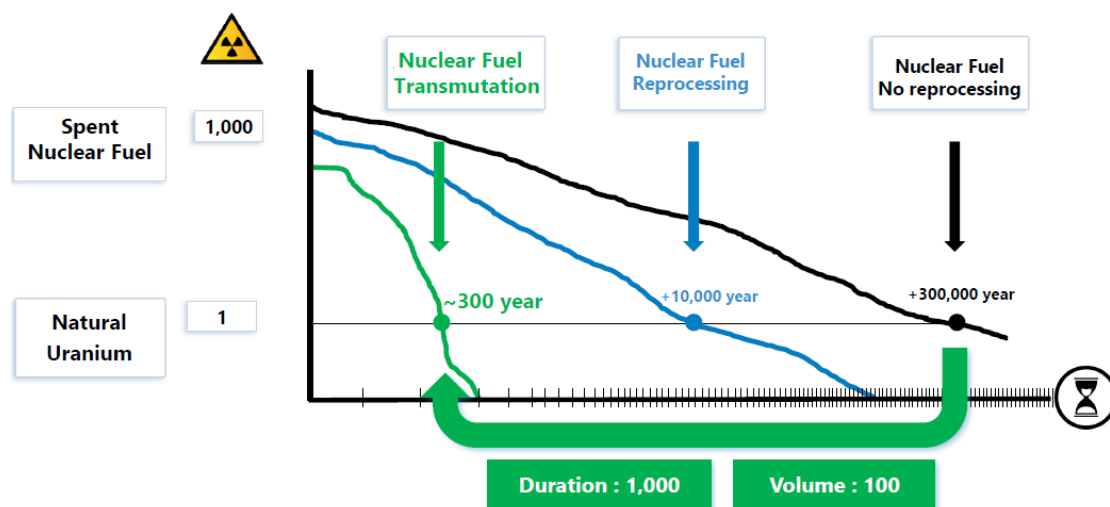


Figure 3 – Evolution in time of the radiotoxicity of the spent nuclear fuel [10]

Nevertheless, in order to reach this objective, specific technologies have to be developed and implemented. As it has already been introduced in the previous paragraphs, a finite number of conceptual innovative designs of nuclear reactors have been identified, all belonging to the new generation of installations named GenIV, in order to answer to the following main constraints and requests [11]:

- Doubling of the electricity consumption foreseen by 2050;
- Sustainable development concerning environmental aspects, such as nuclear radioactive waste management or efficient use of the natural uranium resource;
- Safety and reliability of the systems, as well as a better resistance to proliferation risk;
- Economic competitiveness with regards to other energy sources and technologies.

As it is possible to visualise below in Figure 4, fast reactors will have an important impact on the amount of spent fuel produced compared to the currently operating thermal reactors, because the most harmful elements within contained can be efficiently transmuted under fast neutron flux, in

addition to the advantage of fuel reprocessing, i.e. closed fuel cycle, thus limiting the amount of radioactive waste directly allocated in a deep geological disposal. Additionally, these reactors will also have a better use of the natural existing uranium resource, that is a lower consumption of fresh fuel, contributing to a longer exploitation of nuclear power plants depending on the year of introduction of such fast reactors.

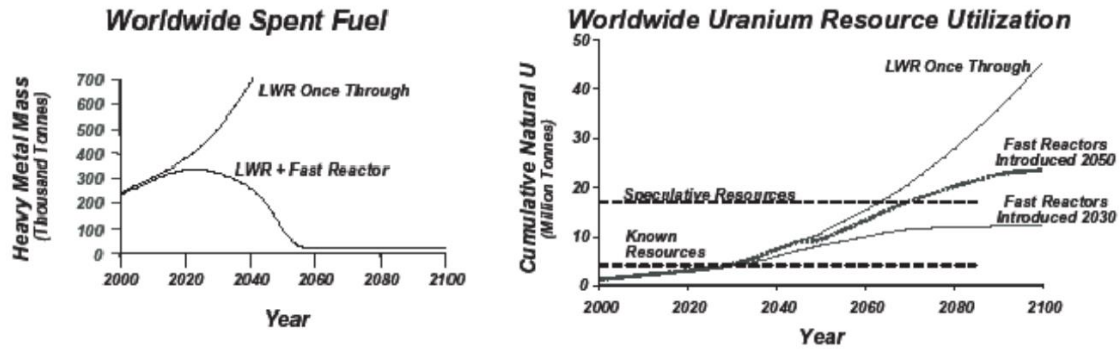


Figure 4 – Impact of implementation of fast reactors on the produced spent fuel amount (left) and the availability of natural uranium resource (right) [9]

Other main desired characteristics for these selected designs are the possibility to work at high temperature to increase the thermal cycle efficiency, and at low pressure to reduce the potential energy stored in the structure and consequent disruptive dispersion of material; possibility to exploit a closed fuel cycle and to have smaller sizes, both for economical purposes (faster return of the investment) and for increased security. However, fast critical reactors have a limitation on the amount of waste they can treat, due to the consequent decrease in controllability and safety.

For this reason, the ADS reactor principle is being introduced [12]. This technology foresees the coupling of a particle accelerator and a nuclear reactor and the concept has been initially proposed as an alternative to the classical critical reactors in the 1950's by Nobel Prize laureate E.O. Lawrence, with the use of a cyclotron, proposal abandoned due to the weak reliability of the accelerator. Later the idea has been further developed by Nobel Prize laureate C. Rubbia in the 1990's, due to the advances in the accelerator systems and it has been applied for the first time to energy production.

The main characteristic of an ADS is the presence of a sub-critical core, that is the inability of the core of self-sustaining the fission chain reaction. Therefore, the addition of a neutron (spallation) source is needed: placed at the centre of the core, it provides the necessary primary neutrons, which are then amplified by the core. Specifically, a heavy nuclei target is bombarded by high energy protons, which are causing a series of direct reactions, i.e. intranuclear cascade,

subsequently leading to the ejection of neutrons in an excited state from the nuclei by direct collision, as shown in Figure 5 [13]. In the latest designs, the protons are accelerated by a LINAC, able to produce the required beam intensity with a reasonably high reliability. It is important to mention that higher the energy of the incident protons and heavier the nuclei of the spallation target, higher will be the number of neutrons produced.

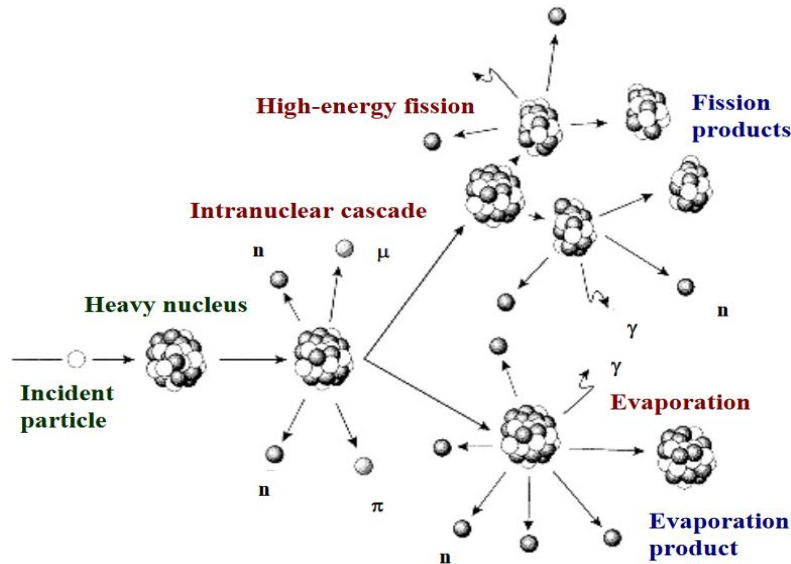


Figure 5 – Scheme of a spallation reaction [13]

This configuration provides the inherently safe feature of these systems, because the reactor is switched off as soon as the proton beam is too. Yet, in case of dangerous conditions, the efficient capability of the decay heat removal must be equally guaranteed. Another relevant implication of such arrangement is the possibility to load either conventional fuel, i.e. MOX or UO₂, or advanced fuel loaded with MA⁴, leading to high and efficient transmutation rates, since reactivity coefficient issues will not be encountered, as it occurs with critical fast reactors. [14]

Indeed, MA loading has an impact on the core physics parameters, namely the delayed neutron fraction β_{eff} , that determines the time-constants for the reactor control, doppler temperature coefficient, that is the reactivity feedback⁵ consequent to a change in temperature in the fuel, and

⁴ These types of fuels are often referred to as dedicated MA bearing targets. The fuel is non-fertile, that is free of uranium, in order to prevent the production of higher actinides through uranium capture, thus, to increase the transmutation performance. Additionally, it contains a high concentration of actinides. [15]

⁵ Reactivity feedback coefficients are parameters that describe the change in reactivity of the reactor subsequent to a change in such parameter. Nuclear reactors must be designed such that they have a negative feedback mechanism, that is, any perturbation leading to off-normal conditions should be counteracted by some feedback, which thus brings the system back to steady-state conditions. [16]

the void coefficient, to with the reactivity feedback resulting from the generation of bubbles inside the coolant. Consequently, a big load of MA can jeopardize the control of critical reactors, because the reduced delayed neutron fraction decreases the margin to prompt criticality, together with a reduction of the doppler feedback effect, leading to unmanageable reactivity induced transients.

Within this continuously developing framework, the MYRRHA project was born in order to demonstrate the feasibility of transmutation of MA through ADS at a semi-industrial scale, and it is presently under an advanced stage of development at the Belgian research centre SCK•CEN.

1.3 MYRRHA reactor project

MYRRHA is the first prototype in the world of a particle accelerator driven nuclear reactor, with a significant thermal output, with very wide and differentiated operational goals. It will not only support research programs of significant European interest: one of its greatest advantages will be the demonstration burning of nuclear waste, i.e. transmutation of highly radioactive fission products, in order to reduce volume and radiotoxicity of radioactive waste [17]. Therefore, a desirable outcome would be the one of an increasing sustainability of nuclear energy, as well as its social acceptability from the population. Nevertheless, in order to do so, the safety assessment of the reactor design is of immense importance, hence the scope of the present work is to contribute to its development.

MYRRHA [18], [19] a flexible fast spectrum research facility, is conceived as an accelerator driven system, able to operate in sub-critical and critical modes. Indeed, as described in the previous section, since in the reactor core there is insufficient fissile material to spontaneously maintain the fission, it must therefore be continuously fed by an external neutron source, which consists of a proton accelerator of 600 MeV. This accelerator fires protons at a compact LBE target, the spallation neutron source, which creates the neutrons that will maintain the fission chain reactions in the reactor, loaded with MOX fuel and cooled by liquid lead-bismuth eutectic.

As visible in Figure 6, the components of the primary loop of this particular pool-type reactor setup, as for example the heat exchangers, pumps and in-vessel fuel handling mechanisms, are

In specific, the void-reactivity feedback is related to any modification of the density of the coolant, which affects the neutron moderation: any decrease in the moderator density leads to a worsening of the neutron moderation. It is clear that any perturbation of the reactivity of the system leads to a perturbation of the reactor power and of the produced heat, which in turn will create a modification of the fuel temperature. This is known as Doppler temperature coefficient, for which an increase of the temperature has for consequence the broadening of the capture and fission resonances. This will further decrease the reactivity, therefore the power produces, bringing the reactor back to a stable condition.

inserted from above through the thick concrete lid. The proton beam originated from the particle accelerator that triggers and maintains the chain reaction, enters the hanging vessel with toro-spherical bottom from the top as well. This technology is safe and easy to control, because the chain reaction will stop automatically by switching off the particle accelerator [20]. This latter element is required to be reliable with an extremely high mean time between failures to have a continuous and powerful proton beam.

As already stated above, MYRRHA is designed as a multi-purpose irradiation facility for fuel testing, material development for both fast fission and fusion reactors, study of transmutation of high-level nuclear waste and the production of theragnostic radio-isotopes, i.e. for diagnostic examinations and therapeutic treatment [5], for medical, but as well as industrial applications.

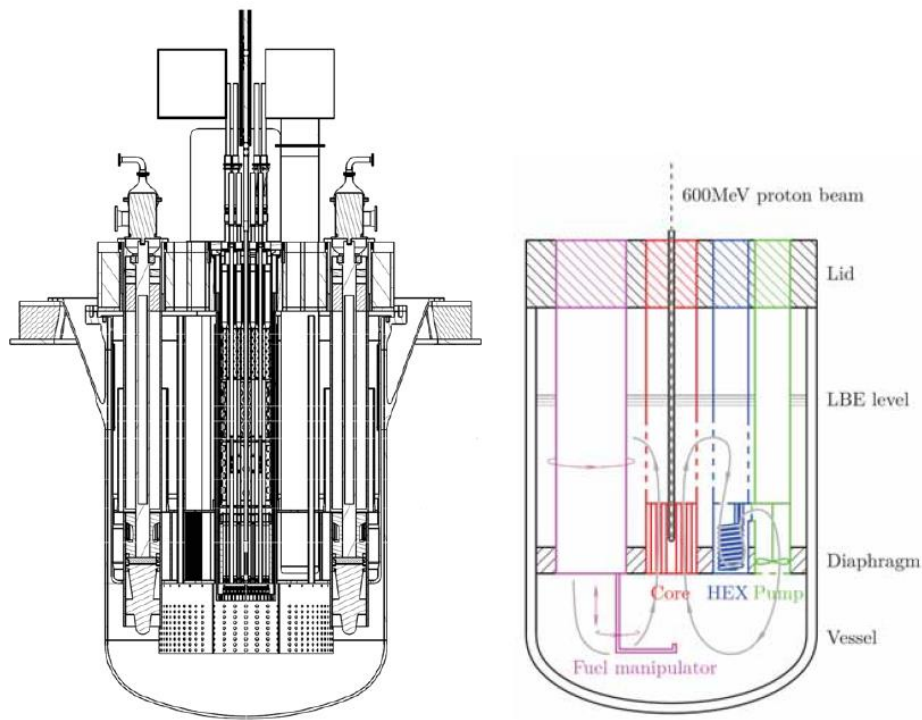


Figure 6 – MYRRHA reactor design [from the MYRRHA Technical-Brochure, 2016]

It belongs to the family of LFR [21], and as such, its fast spectrum enables a better resource utilization by means of the low-moderating and low-absorption operating fluid (LBE), as well as a waste minimization and management through transmutation of the minor actinides. Compared to the other concepts, this design is simple and compact, because lead doesn't react neither with air nor with water and owing to the very low vapor pressure of lead, operation is possible at atmospheric pressure. The low likelihood and degree of core damage is achieved thanks to the high thermodynamic properties of the coolant, namely heat transfer, specific heat and thermal

expansion coefficient, as well as to the core's inherently negative reactivity feedback, i.e. negative void coefficient. Consequently, the fuel pin pitch is larger, allowing for lower pressure drops and the possibility to remove the decay heat via natural circulation, also thanks to its good thermal expansion. Further reactor safety and reliability is addressed on account of the coolant density close to the one of the fuel, guaranteeing a reduction of the risk of re-criticality in case of core melt, because the fuel will rise upwards due to buoyancy and spread on the free surface of the fluid instead of collecting at the bottom of the reactor pressure vessel, hence not generating a critical mass (mass of fuel required in order to reach criticality).

As far as the core configuration is concerned, it is composed by a cluster of hexagonal-shaped fuel assemblies, each containing 127 fuel pins with a 15-15Ti⁶ cladding and wrapped in an helicoidal wire spacer. The core is then contained in a pool-type reactor vessel, in which the upper hot zone is separated from the lower cold one by a diaphragm and where the cooling LBE flows in forced convection, pumped through the core from the lower plenum. In normal operating conditions at 100 MW_{th} core full power the fluid works at atmospheric pressure and at relatively low temperature, achievable thanks to its reasonably low melting temperature (123°C): the inlet core temperature is 270°C, outlet core temperature equal to 350°C [23]. The hot liquid metal then enters the core barrel, that is a big pipe above the core in which several holes have been made to have a better distribution of the fluid in the upper plenum, and it is finally cooled into four heat exchangers, in which the thermal power is removed by water.

As already mentioned, the MYRRHA reactor is also intended to run as a critical fast neutron irradiation facility, with decoupling the accelerator and removing the spallation loop from the reactor core [24]. This means that the design considering the sub-critical mode operation has to be modified, and that reactor control and scram systems have to be included. As a matter of fact, two reactor shutdown systems have to be added to guarantee diversification, one of which will function as control system. Secondly, the changes in the design have to consider that the critical mode operation will significantly have an impact on the safety characteristics of the facility, therefore the effect of the safety feedback on the design needs to be implemented. [25]

Hence, LBE is one of the most critical elements of MYRRHA, which accordingly will also have to prove its feasibility to be used as both nuclear coolant and spallation target material.

⁶ The cladding material that will be used in the MYRRHA reactor is a titanium stabilised austenitic stainless steel. The addition of Ti as stabilizing element showed an enhanced resistance to void swelling and creep strength compared to other stainless steels, thus presenting more advantageous properties in its use as cladding material. [22].

1.4 Lead-Bismuth Eutectic as nuclear coolant

The choice of LBE as specific nuclear coolant for the innovative nuclear research facility MYRRHA is because this liquid metal meets most of the required conditions, such as advantageous material properties, neutronic and thermophysical characteristics. It is a eutectic with composition of 55.5 wt.% Bi and 45.5 wt.% Pb. [26]

Together with the advantages and properties that are already been introduced in the previous section, LBE has other interesting characteristics, like the high boiling temperature (1671°C) that allows for an enhanced margin to safety, the possibility to use it as neutron reflector, which leads to an increased efficiency in the neutron economy together with its low neutron absorption cross-section. These properties are of major importance also in the use of LBE as spallation target, since as such it is subject to extreme conditions like the high beam energy deposition in its relatively small volume. Its high density and atomic number enable this fluid to achieve a high neutron yield, i.e. the large production of neutrons per spallation reaction, aspect which is contributing to the choice of LBE as suitable spallation target. [27]

Among the excellent thermo-physical properties of the liquid metal of interest it is possible to highlight the high thermal conductivity, which guarantees for an increased heat transfer efficiency, the high specific heat capacity, that allows for an enhanced cooling of the system and effective heat evacuation both in normal operating condition and in transients regimes. [28]

Additionally, as LBE is compatible with water, the required chemical inertness is attained, allowing for the use of the latter as secondary cooling fluid, without the need of intermediate loops. [29]

Nonetheless, this coolant presents some drawbacks as well: it is opaque, thus remote fuel handling and ultrasound visualization are needed. Limits on the fluid speed (2 m/s) and the cladding temperature must be established, due to the issues related to erosion and corrosion of the most common stainless steels by LBE [28]. An additional major issue is the behavior of LBE under irradiation. Indeed, LBE becomes highly radioactive due to the production of a series of harmful radionuclides, resulting from the activation of the isotope Bi-209 into Po-210 during the spallation process. Hence, the elevated radiotoxicity and relatively high volatility of the Po isotope resulting by this neutron capture reaction poses a concern on the use of LBE in such nuclear facilities [30]. Moreover, the lack of experience in previous operating technologies and its expensiveness, as well as the rareness, are among the main disadvantaged in the use of LBE.

In conclusion, given that there is no material that meets all the required criteria and that the selected one, which acts both as coolant and as spallation target, has necessarily been a compromise among all the aforementioned aspects, the present analysis will primarily focus on the safety concerns linked to the cooling capacities of this fluid in accidental scenarios. More specifically, the case in which unforeseen blockages obstruct the subchannels of the fuel assembly will be considered.

1.5 Fuel assembly blockage

The fuel assemblies of MYRRHA have a similar design to previous fast reactor fuels and consist of a hexagonal tube with a tight packed triangular lattice of fuel pins. To maintain the relative position of the rods, each one is wrapped with a helicoidal wire, which also keeps the distance from the neighboring rods and the hexagonal tube.

As already anticipated, in off-normal operating conditions foreign particles might pollute the coolant LBE, subsequently forming possible local obstructions to the flow within the rod bundle. Additionally, depending on the origin of such particles, the shape and porosity of the blockages can be different. For example, they could be caused by single pieces of debris or by build-up of particulate matter [31].

Although after the lesson learned from the Fermi I accident [32] all nuclear facilities of this type have specific fuel assembly inlet flow paths in order to prevent complete blockage of a subassembly, envisioned to not allow entry of foreign material, the buildup of foreign matter in the smallest flow paths of the fuel subchannels could still represent a risk caused by the formation of different sized blockages. The consequences of such blockages on the system depend on several factors, like their size, material, location or distribution, that is either a local concentration or distributed over several subchannels of the fuel assembly [33]. Indeed, in the severe case of several blocked contiguous channels, the temperature of the fuel in the heated zone might reach unacceptable values, also due to a reduction in the flow in that area, phenomena that constitutes a problematic issue regarding safety, since it is not always easy to detect, being the increased pressure drop due to partial blockages small compared to the pressure of the complete fuel assembly.

The origin of the blockages might be very heterogeneous: they can be caused by lodged debris in the fuel subchannel, accumulation of fragments of broken wire-wrap spacers, swelling of fuel pins either due to defects or weak spots, or due to over-enriched pellets, or poor heat transfer caused eventually by gas release or distorted pins [31]. Specific to lead-cooled reactors are

accumulation of structural material corrosion products and of broken wires, in addition to possible coolant subchannel flow area reduction due to cladding deformation under irradiation. [34]

In the most undesirable scenario in which the fuel particles are originating from a cladding failure, the blockage might even generate heat.

For the reason that it is assumed that these obstructions could have a negative impact on the heat transfer from the fuel to the coolant, all the above cases have been postulated as potential accident initiators and are being therefore investigated, particularly with respect to their potential for failure propagation.

1.6 Safety aspects and requirements

Nuclear power is generally considered as sustainable energy source, since throughout its life cycle, the emission of polluting gases is comparable to the RES [35]. In addition, it is a stable source and mature technology, as well as reliable and efficient [36]. However, the safety of energy supply is of underlying importance, and many concerns have risen regarding this matter [37], most of them raised after nuclear disasters. Furthermore, nuclear fuel and wastes are highly radioactive, posing many threats to public health and the environment, because it involves mining and refining of radioactive raw materials [38]. It is important to mention that this latter aspect is marginally considered when it comes to the discussion of the impact of nuclear power to the population: the mining and enrichment process, that require transportation of the radioactive material put the population under increased risk for cancer and other health problems due to long-term exposure to low-level radioactivity. Ethically speaking, these actions go against the principles of nonmaleficence and justice, since there is a lower chance of inflicting the least harm possible to reach a beneficial outcome only to the local residents. Hence, a secure energy supply is thus not simply a technological or economic matter, but rather a political and ethical question [39].

The recent nuclear disasters have generated different issues globally impacting on public health, environment, and psychosocial effect, generally because nuclear power plants are located in densely populated areas, thus ultimately causing public fear towards nuclear power [40]. This leads to a not so favorable public opinion, and this could contribute to mine the future development of nuclear facilities. In order to avoid this eventuality, it is therefore of major importance to address the safety related to the different operational aspects, because it is a keystone for the licensing of nuclear installations.

Within this regulatory context, MYRRHA is classified as “Class I facility”, which is the one characterized by the highest hazard level, and it has to go through the pre-licensing process with the supervision of the Belgium regulatory authority for the safety of nuclear facilities FANC in order that the feasibility of the project is ensured. The several objectives of the pre-licensing phase include the identification of potential safety issues that could jeopardize a license application, the development of the objectives for safety and security of the installation, as well as development of answers and justifications to specific nuclear safety issues. [18]

As MYRRHA follows the principle of defence-in-depth, a series of legally and non-legally binding references will be used in the nuclear safety approach, incorporating the most advanced and stringent requirements. In specific, these recommendations come from the Belgian regulatory framework and European directives, as well as the IAEA safety standards, the FANC regulatory guidelines, the WENRA safety reference levels and the NRC guidelines, respectively.

As the application of the IAEA specific safety requirements are concerned, the IAEA fundamental safety principles SF-1 have been adopted for the development and the design of MYRRHA components, and the principal technical requirements are listed in Table 2, where the challenges present in the second column are related to the introduction of innovative design features, and that have to be solved in order to comply with the requirements and to demonstrate the safety of the facility [41].

Req. 5 – Radiation protection in design	Choice of LBE as a coolant and the generation of Po-210 with respect to safety of the workers during maintenance operations
Req. 9 – Proven engineering practices	Qualification of thermo-hydraulic codes for the use of LBE as coolant
Req. 7 – Application of defence-in-depth	Understanding the properties of LBE as a barrier for activation and fission products
Req. 6 – Design for a nuclear power plant	Increase in design, construction and operation experience of technologies of the facility
Req. 10 – Safety assessment	Increase in safety assessment methods to investigate postulated accidental sequences
Req. 7 – Application of defence-in-depth Req. 9 – Proven engineering practices	Investigation of the long-term effect of LBE on material properties
Req. 4 – Fundamental safety functions	Effect of LBE freezing temperature on the fluid flow

Table 2 – IAEA principal technical requirements

These challenges are faced through extensive R&D programs and experimental facilities in order to investigate the feasibility of the introduction of the innovative design features and to meet the required acceptance criteria and set the necessary operational margins. Among these, some other additional challenges are currently explored to evaluate the safety requirements of the plant design, like [42]:

- *Req. 16* – Postulated initiating events. The identification of initiating events is based on methods that rely principally on a detailed knowledge of the technology of the installation and the physical processes that regulate its work, and these are used to evaluate the impact of such events;
- *Req. 17* – Internal and external hazards. Although the classification of external and internal hazards is not specific to MYRRHA, certain risks like the potential of flooding a cavity with LBE containing volatile polonium must be identified. It is indeed important to detect all the possible causal coincidence of different external hazards and of external and internal events;
- *Req. 19* – Design basis accidents. As for all the existing fleet of nuclear facilities, a list of design basis accidents must be identified, whose analysis will then be used to specify the performance criteria of all the safety systems;
- *Req. 21* – Physical separation and independence of safety systems. As far as the DiD is concerned, a series of principles are investigated in order to guarantee the independence between different lines of defence. Among these, the use of passive systems is included, as well as lines of defence that hinder the onset of common mode failures and of multiplicity of systems inoperability;
- *Req. 25* – Single failure criterion. The acceptable mitigation of the aforementioned design basis events and anticipated operational occurrences will be demonstrated by the application of the single failure criterion during the safety demonstration.

As already mentioned above, within this framework of analysis and the implementation of all the required safety criteria, several fundamental research programs have been established to tackle the defined challenges related to the introduction of innovative design features. Hence, different experimental facilities have been built for equipment qualification, as well as numerical simulations have been performed, all in order to demonstrate the safety of the facility. According to this regards, in the next chapter the focal points of the experimental campaign performed at the THEADES loop of KIT-KALLA and the numerical assessment developed by

the internationally operating nuclear service provider NRG, both within the framework of the European Project MAXSIMA, will be presented, whereas the complete detailed information could be found in the reference [43], [44], [45], [46] and in “Appendix A – Detailed description of the background experimental campaign and numerical simulation” of this thesis.

1.7 Aim and organisation of the thesis

The objective of the present work is the development of a CFD model within the framework of the forced-convective studies linked to the heavy-liquid-metal thermal-hydraulics in the MYRRHA fuel assemblies. The purpose is indeed the analysis of the flow behavior of LBE in accidental conditions, in order to evaluate the safety assessment of such technological design in the unfavorable case in which subchannel blockages are present.

More specifically, the goal of this thesis is to build a model of the 19-pin wire-wrapped fuel bundle with blockage so as to investigate the effect of porosity and self-heating of such blockage on the temperature distribution within the fuel bundle. In order to so, an in-dept review of the already existing experimental and numerical data has been done, which can be found in “Chapter 2 – ” as further explanation of the scope of this analysis and comparison of the obtained results.

Subsequently, the core of the work focuses on the methodology of the CFD model development for the evaluation of the subchannel and cladding temperatures using the commercial CFD code ANSYS CFX, whose theoretical basis regarding turbulence modeling will be described in “Appendix B – Numerical modelling theory”.

The structured investigation of the different modelled systems, like the domain geometry, the choice of meshing technique as well as turbulence models are thoroughly explained in “Chapter 3 – Fuel assembly model without blockage”, “Chapter 4 – Fuel assembly model with solid blockage”, and “Chapter 5 – Fuel assembly model with porous blockage”, where also the modelling of the blockage geometry and its properties, as the porosity, thermal conductivity and power, are studied in order to estimate the safety significance and effect of the postulated blockage accidental scenario.

1.7.1 Verification and validation

The objective of the present work is the validation of the CFD method against experimental data and previous numerical simulations for the prediction of the temperatures in blocked fuel bundles, as well as further code validation for porous blockage in preparation of the experiments. In fact, this work is part of the set of preliminary studies in support of the design and licensing of the MYRRHA reactor. As mentioned before, it is an accelerator driven system, cooled by lead-

bismuth-eutectic, which is a liquid metal coolant with the already described interesting and peculiar characteristics. Given the introduction of these innovative features, there is the need to assess the safety of the installation by studying the performance of the primary cooling system also in accidental conditions. In order to do so, for the specific case under analysis, several experiments and numerical simulations have investigated the consequences of flow blockages in a fuel assembly, which the thesis has been compared to in order to perform the validation of the results. In fact, with this process it is possible to build numerical models which are representative of the reality, and once it is proven that they properly describe the occurring physical phenomena, it will be possible to simulate every possible scenario, whichever the complexity of the system and combination of features and parameters.

Chapter 2 – Background of the work

Taking into account the specific field of applications considered, numerical CFD models are developed in order to investigate the thermal hydraulic behaviour of these innovative reactors in nominal, as well as accidental conditions. The objective of the development is to establish a tool with which it will be possible to predict in a reliable way the most important occurring physical phenomena, and therefore to simulate efficiently changes of the reactors, both in the design and in the operational thermal behaviour. In this way the obtained results can support the design and safety analysis of the liquid metal-cooled reactors. [47]

In this context, the reliable modelling strategy and a profound validation of the numerical approach has to be performed, to analyse the performance of lead-cooled fuel assemblies and to predict accurately the limits to the safe operation of the reactor [48]. In fact, CFD methods are a quite convenient way which can provide a detailed thermohydraulic flow profile inside the rod bundle, together with the precise evaluation of local velocities, temperatures and hot spots location, possibility which is limited for physical measurements.

For this reason, since complexities in heat transfer modelling of low Prandtl number fluid flows arise due to the separation of the viscous and the thermal length scales, there is a clear need for validation, adaptation or development of the turbulence models. In this view, experimental investigations on thermal hydraulics of liquid lead alloy are performed for development of accurate models [49].

In particular, as it has been shown by accidents leading to fuel element cladding damage occurred in the past like in the SRE and Fermi-1 sodium-cooled reactors [50], the presence of internal blockages in fuel rod bundles is a probable postulated event. Partial flow blockage of coolant channels is a dangerous event that can jeopardise the safety of the reactor: when the fuel assembly is partially or totally blocked, the heat transfer between coolant and cladding is significantly degraded due to a local rapid decrease of coolant flow, leading to the generation of hot spots that can possibly results in a fuel pin failure. [51]

Regarding the lead-cooled reactors, they generally adopt wire-spaced bundles, therefore the accumulation of debris from failed fuel pins or broken wires is generally expected to occur along the wire. Hence, in this case, the preferential shape of the blockage develops along the axial direction and it follows the helicoidal wire. This behaviour is in complete opposition with grid-spaced fuel assemblies: the experimental results obtained on blockage growth by particles show

that these are collected at the spacer grid, thus a horizontal blocking plate with strong radial growth tendency is created. [52]

More specifically, the partial blockages that are likely to occur in these reactors are of two types: global or local. At a global level, partial blockage at the fuel assembly foot may be caused by foreign materials left during construction [51]. In this case, the mass flow rate is reduced due to the higher pressure drop encountered. For this reason, fluid and cladding temperatures rise, due to the lower velocity and hindered coolability of the rod's surfaces. Nevertheless, in the current innovative reactor designs mechanisms to detect such occurrences are present. Indeed, the temperature at the hottest locations and at the outlet can be evaluated in an integral analysis based on correlations developed for an unblocked assembly, minding the neutronic feedback on the thermal power. [50]

On the contrary, at the local scale internal blockages can be originated by ingress of foreign material, corrosion products as well as broken wire, which may accumulate in the flow channels. Besides, an even more dangerous situation is the build-up of debris from failed fuel pins, because of the additional release of heat. As mentioned before, the heated wall cannot be cooled efficiently, leading to local hot spots. These are instead more difficult for the protect system to detect the local flow blockages, because of their negligible effect on the total mass flow rate or mean velocity. Consequently, local flow blockages cannot be detected efficiently by the increase of pressure drop of outlet temperature. [53]

This latter mentioned eventuality is considered to be one of the important issues to be addressed, because the lack in prompt detectability during operation of such obstructions can lead to damage propagation. Yet, although the importance of investigating the underlying phenomena caused by them, the complex mechanisms involved make the accurate assessment of their consequences challenging. For this reason, several experiments and researches have been carried out to investigate the flow and heat transfer process in wire-wrapped rod bundles. The main aim of these studies was the derivation of empirical correlations for pressure drop and heat transfer to be employed in numerical codes, and the current CFD techniques, which are increasingly used for the assessment of wire wrapped fuel assemblies, need for experimental validation at detailed level [54]. Indeed, the obtained results can be employed to prove the correctness of the numerical configuration and to continuously improve the modelling methods.

It is nevertheless important to mention that the use of the modern CFD techniques in the modelling of the thermal hydraulic accident analysis at fuel assembly level is still limited. This is because

often the computational grid refinement needed for accurate predictions cannot be achieved if a complete fuel assembly has to be modelled in detail. Therefore, in order to reduce the amount of computational effort and to maintain a reasonable accuracy, low resolution or under-resolved meshes are used, in which also the geometrical representation of the rod bundle and of the fuel assembly as well is simplified. [54]

Unfortunately, in the field of CFD simulations, studies on the above-mentioned situations of off-normal conditions are still narrow and need to be further developed for the design and safety assessment of wire-wrapped fuel assemblies. Indeed, validation of engineering CFD methodologies should be based on a combination of comparisons to experimental and numerical reference data. This is because the experimental data allow for comparison to physical phenomena, but they are limited in resolution and measurement possibilities, in addition to the eventual uncertainties in geometry and boundary conditions. On the other hand, the numerical reference data allows a well-defined assessment of flow and heat transfer with respect to geometry and boundary conditions at every location in the domain [55]. It is in this framework that the present thesis and the below explained experimental and numerical background are established.

2.1 Experimental background

In the frame of international cooperation, MYRRHA like-bundle experiments also including representative blockages have been performed at the THEADES loop at the Karlsruhe Institute of Technology (KIT). In particular, such experimental campaign evaluated the effect of the introduction of blockage elements inside the already existing setup of the hexagonal-shaped 19-pin wire-wrapped fuel assembly exploited within the European FP7 SEARCH project [56]. Therefore, the outcome of this study will show the difference of the blocked scenario compared to the undisturbed one, although its principal goal is to provide reliable information for the safety assessment of LBE cooled systems, establishing the maximum wall superheating occurring in the accidental condition of partial flow blockage. [43][44][45]

2.1.1 Test section

As already mentioned above, the test section that has been used to perform the experimental campaign with the blockage elements is the reference hexagonal flow channel containing the 19-pin wire-wrapped rod bundle, a scaled-up version of the MYRRHA fuel assembly for practical technological reasons: 45% larger heated length and 25% larger rod diameter and pitch, whereas the geometrical ratios P/D and H/D are constant (see “Appendix A – Detailed description of the background experimental campaign and numerical simulation” for the geometrical parameters).

In Figure 7 both the side view of the complete test section and top view of the fuel rod bundle are visible. It is separated in two sections: the first is a relatively long cold zone, after which a fully developed velocity profile is entering the downstream heated second portion. Here three measuring levels (MLs) have been identified, where most of the instrumentation has been installed on three identical 60° sectors, at which only the relative position of the wires differs (60° rotation of the wire every sixth of the wire pitch).

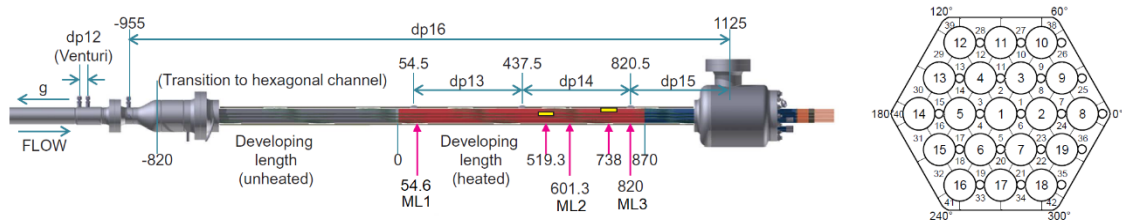


Figure 7 – Side view of the complete test section (left) and top view of the cross-section of the fuel rod bundle (right).
Blockages are represented in yellow [44]

Indeed, the thermocouples (TCs) are placed both at the rod wall and at the centre of chosen subchannels in order to obtain very detailed experimental data on the temperature development through the test section and the localisation of the hot spots, as showed in Figure 8.

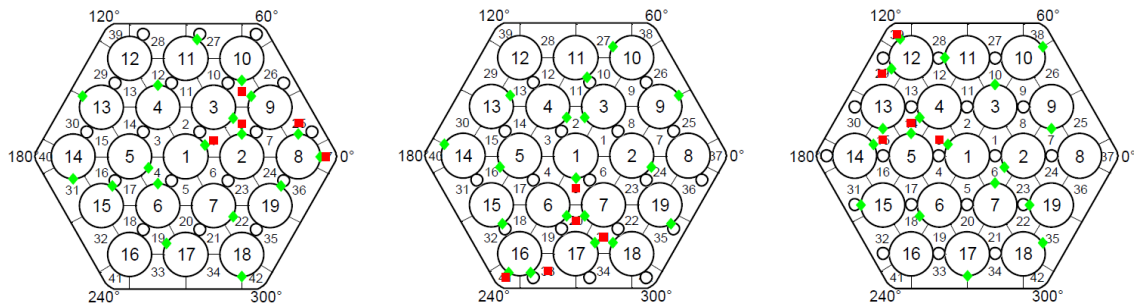


Figure 8 – Top view of the sub-channel (red) and cladding wall (green) thermocouples location installed at ML1 (right), ML2 (centre), ML3 (left) [58]

Detailed information regarding the blocked experiments is coming from the installation of thermocouples located both in the neighbouring rods in correspondence to the mid-height of the blockages, where the hottest points are expected to be, and in their wake region (see Figure 9).



Figure 9 – Position of the thermocouples installed at the blockages mid-height and in the blocked subchannel in their wake region (C1 on the left and E1 on the right) [45]

As far as the temperature measurement is concerned, as already anticipated above, it is done using thermocouples. These have been calibrated, with a resulting precision of 0.1 K [45]. It is important to mention, without entering the specific details of the data sampling procedure, that the digital resolution of the instrumentation led to a step of 0.076 K for the TCs, indicating that a minimum uncertainty of ± 0.038 K in the reading of the signals must be considered. In conclusion, the experimental temperature values, which are also then used for the comparison with the numerical results of this thesis, are presented with a ± 0.10 K uncertainty. [45]

2.1.2 Description of blocked setup

Given the peculiarity of the fuel assembly design, it was concluded that these postulated accidental scenarios are expected to have extended blockages in the axial direction, because of the higher likelihood of debris accumulation phenomena, with a big variety of parameters characterising them. For clear practical reasons, the variables which could be acted on have been reduced, hence only a restricted number of scenarios have been tested.

Established that the worst-case scenarios must be investigated, and that the technical construction feasibility must be taken into consideration, two different setups have been implemented. For both situations the blockages are limited to one sixth of pitch length, due to the practical difficulties in their manufacturing presented by the wire, and are constituted by a low conducting material encased in a thin-walled stainless steel shell to allow the insertion of the blockages in the bundle, hence completely solid. In both the setups. The blockage element geometry is such that allows their insertion in the subchannels, therefore they are fabricated in compliance to the subchannel geometry and the wire presence as depicted in Figure 10.

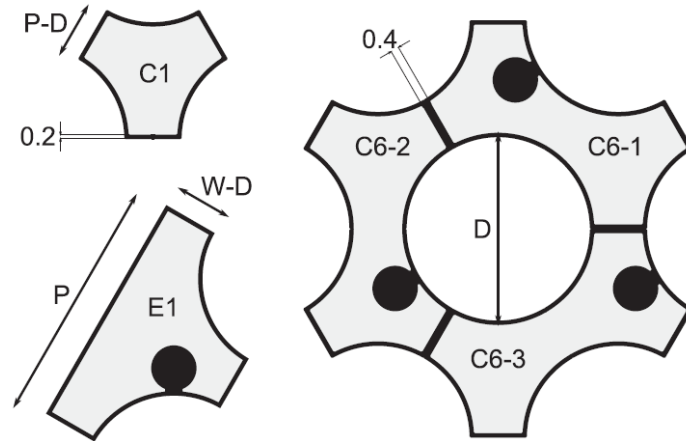


Figure 10 – Blockage geometry: 0.2 mm thick metallic shell (dark) filled with low thermal conductivity ceramic paste (light), crossed by the wire (black circles) [50]

Depending then on the case considered, the size and location of the blockages varies: the first one foresees the simultaneous presence of two blockages, one central (C1) and one at the edge (E1), obstructing only one subchannel, whereas in the second scenario the blockage will clog the six central subchannels (C6), as represented in Figure 11. In all cases, the blockages have been installed sufficiently downstream with respect to the onset of the heated section to allow the flow development, and the distance between C1 and E1 has been evaluated by preliminary CFD simulations [46] to be enough to guarantee the negligible reciprocal effect on temperature and velocity.

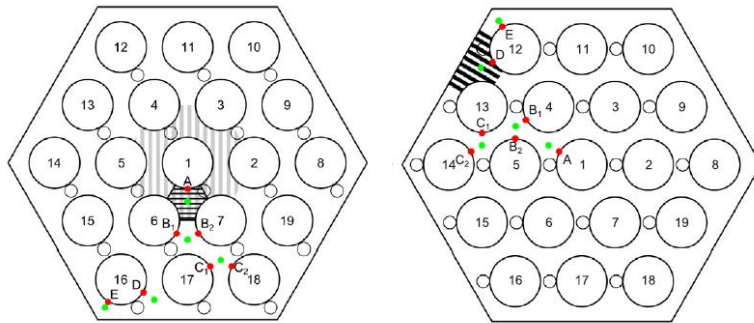


Figure 11 – Top view of the cross-section of the fuel rod bundle: blockage C1 (black) and C6 (grey) at ML2 (left), E1 (black) at ML3 (right) [50]

2.1.3 Test operating conditions

Three parameters were used to define the several investigated operating conditions: inlet temperature, mass flow rate and power. In order to allow the comparison with the data collected in the previous un-blocked experimental campaign, the variables were set in order to obtain the

same conditions, always taking into consideration the operating limit of the THEADES loop, namely maximum outlet temperature equal to 450°C. It is important to specify that the reference case (Table 3), represents the case where the same wall heat flux and Reynolds number as in the nominal operating conditions of the MYRRHA fuel assembly are reached.

<i>Nominal experimental conditions</i>	
Inlet temperature ($T_{in,ref}$), °C	200
Thermal power (Q_{ref}), kW	394
Heat flux ($q_{w,ref}$), MW m ⁻²	0.93
Mass flow rate ($\dot{m}_{ref}$), kg s ⁻¹	18.7
Mean fluid velocity (u_{ref}), m s ⁻¹	1.74
Reynolds number ($Re_{d_{h,bdl,ref}}$), -	44300
Péclet number ($Pe_{d_{h,i,ref}}$), -	1020

Table 3 – Parameters of the reference condition testing scenario [50]

The results for this reference case are discussed in the next section, where only the temperature distribution for the first scenario with the simultaneous presence of the small blockages will be displayed, since they will be the used as reference data for the CFD results obtained in this thesis.

2.1.4 Experimental results and remarks

As could be expected, fuel assembly blockages causing the obstruction of the coolant flow paths lead to the local degradation of the heat transfer, hence a rise in temperature. Such temperature increase is pronounced by the low thermal conductivity of the material, yet it can still be acceptable in the case of single subchannel blockages, because they would not lead to cladding failure. Indeed, the fluid temperature rises locally at the rod cladding surface, due to the presence of the constant heat flux and the reduced velocity, eventually resulting in the onset of hot spots due to the lack of efficient cooling, aspect confirmed by the temperature values given by the TCs located behind the wire. It is also important to mention that given that the rod bundle is encased by an adiabatic hexagonal channel, the edge blockage leads to a larger overheating, whereas for the central one the presence of cross-flow from the neighbouring sub-channels reduces this effect. Nevertheless, the common aspect is the conduction dominant heat transfer within all solid blockages, which lead to a temperature distribution principally peaked towards their centre, aspect confirmed by the TCs at the interface between the rods and the blockages, where the largest temperature overhear is recorded.

Going further in detail for the first blocked scenario, the temperature values recorded by the different TCs at the blockage mid-height, in the downstream wake region and at the measuring levels, are showed in Figure 12, Figure 13, Figure 14 respectively, for both the considered blockages, where the dashed line represents the bulk temperature $T_b(z)$ evaluated as in Equation 1:

$$T_b(z) = T_{in} + \frac{z}{L_{heat}}(T_{out} - T_{in}) \quad (1)$$

It is clear from the figure below that the temperature overhear is depending both from the heat transfer with the materials, that is the temperature values are lower where the surface is cooled by the coolant, and from the presence of the wires, since they act as cooling fins for the low-conducting blockage elements.

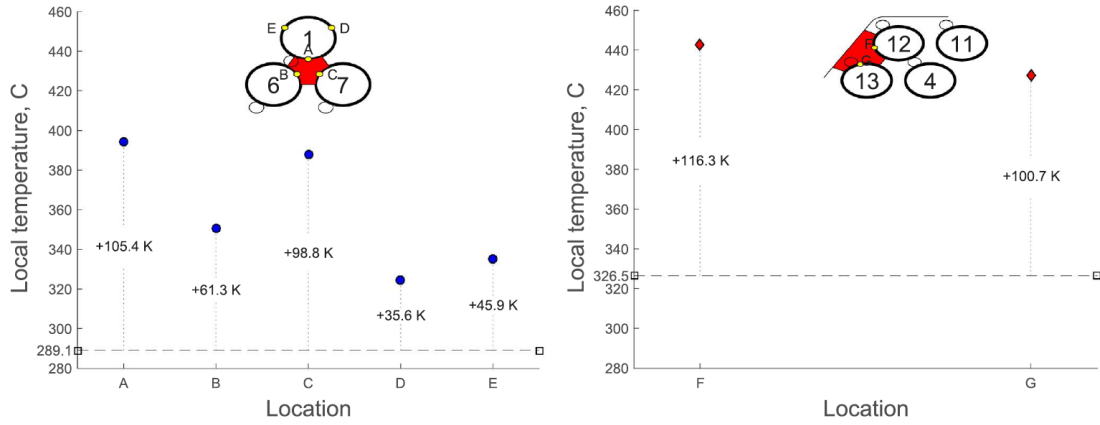


Figure 12 – Reference case temperature distribution at C1 (left) and E1 (right) blockage mid-height [50]

As expected, the linear increase of the bulk temperature indicates the heating up of the fluid along the fluid bundle. From the figure below it is clear that the fluid subchannel temperature profiles in the wake downstream the blockages have different trends: for C1 it is relatively constant, whereas it is non-monotonous for E1, phenomena possibly explained by the change in local velocity.

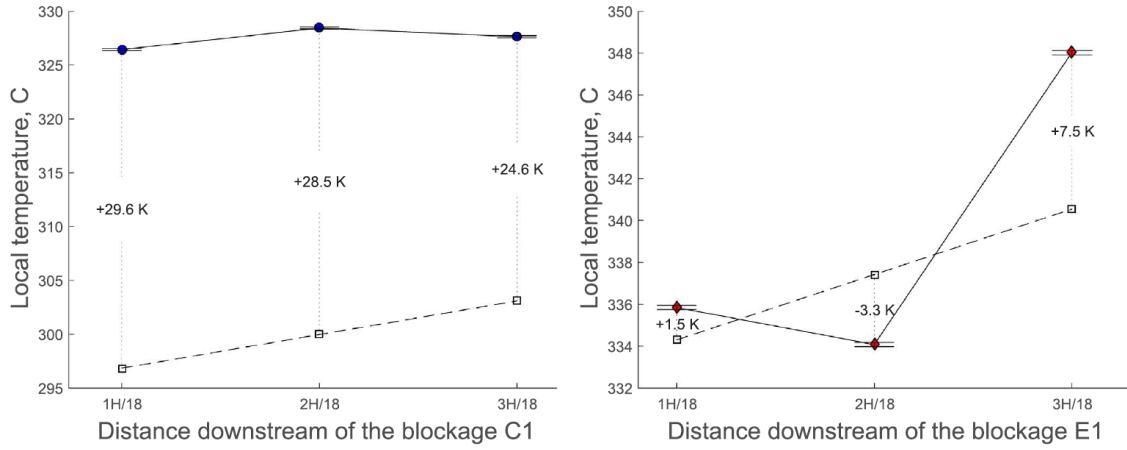


Figure 13 – Reference case temperature distribution in the wake region of C1 (left) and E1 (right) [50]

In conclusion, the set of data recorded at the measuring levels depict a hotter inner region compared to the outer, where evidently the hottest locations occur at the central pin and adjacent subchannel. This fact confirms that the impact of the small blockages is limited to a narrow region downstream them, therefore not constituting major concerns for the safety assessment of the system.

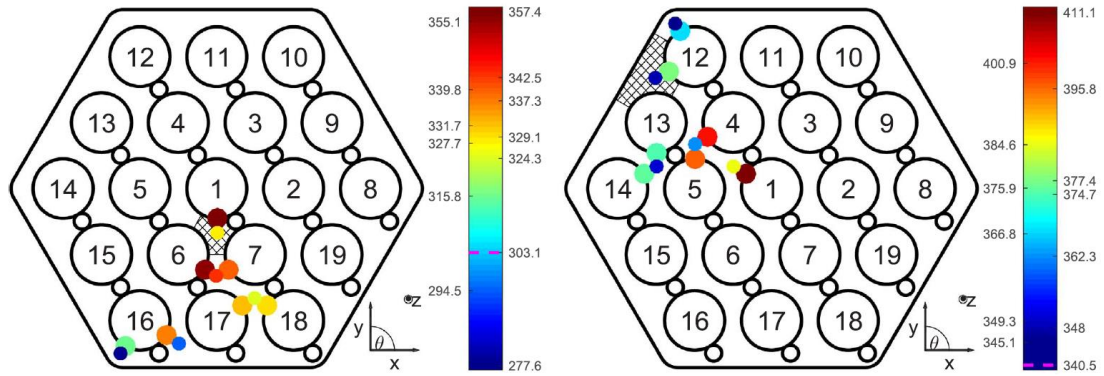


Figure 14 – Reference case temperature distribution downstream C1 at ML2 (left) and downstream E1 at ML3 (right) [50]

Nevertheless, the drawback is the small global effect of such blockages on mass flow rate: the pressure drop increases only partially (total losses increase in the test section equal to 1.2% [50]), as similarly occurs for the outlet temperature, which makes their prompt detection difficult, potentially leading then to worse consequences.

2.2 Numerical background

As anticipated in the 1.7 of this thesis, a very detailed numerical assessment has been performed by the partner institute NRG on the reference solid blockage configurations in the 19-pin wire-wrapped rod bundle representative of the MYRRHA design, experimentally studied at KIT-KALLA (see section above). Particularly, CFD simulations have been developed both as pre- and post-test analyses using the commercial code STAR-CCM+. Indeed, for the purpose of contributing to the assessment of the safety aspects of such system, the goal of former investigation is to assess the feasibility of the experiments and to give a preliminary insight of the effect of low coolability in a blockage accidental scenario, relative to the flow recovery, pressure drop, expected and maximum temperatures at the cladding surface, as well as blockage material. On the contrary, the latter has been developed to understand the uncertainties in the experiments and to validate the numerical model. Therefore, also a series of sensitivity studies has been conducted, in order to define the origin of the discrepancies encountered between the experimental data and the numerical results. Since the scope of the present thesis is not to extensively report the complete analysis made, which could be found instead in the reference [46], only the results of the post-test simulations will be presented below.

2.2.1 Computational setup

The computational domain is based on the first experimental setup, in which the two single sub-channel blockages are studied, and it is constituted by the heated length and two unheated zones (upstream and downstream), with sufficient space provided between the last measuring level and the outlet boundary in order to avoid any influence of the boundary condition on the results.

It is clear that the geometrical dimensions are the same as the ones of the experimental campaign design and they are reported in Figure 75 (“Appendix A – Detailed description of the background experimental campaign and numerical simulation”), together with the sketch of the shape of the wire adopted, which differs from the one used in the CFD model developed in this thesis.

The computational conditions are covering two cases selected among the performed experimental tests, the first (referred as nominal flow rate case) of which represents the nominal operating conditions of the MYRRHA reactor, as far as heat flux and Reynolds number are concerned, whereas the second (referred as low flow rate case) corresponds to the lowest mass flow rate achievable with the same heat flux without damages to the experimental loop.

Table 4 summarises the main information for the computational setup, including boundary conditions, meshing technique, as well as resolution models.

Methods	RANS, standard k-ε model, high y^+ wall treatment, Turbulent Prandtl number ⁷ = 2		
Scheme	Second order segregated flow and segregated heat transfer		
Time dependence	Steady state		
Meshing strategy	Polyhedral cells with near wall prism layers		
Mesh properties		<i>Nominal flow rate case</i>	<i>Low flow rate case</i>
	<i>Total n# cells</i>	15.5e6	9.0e6
	<i>Fluid n# cells</i>	8.1e6	3.5e6
	<i>Avg y^+ rods-wires</i>	47	47
	<i>Avg y^+ channel</i>	51	44
Boundary conditions	Inlet	<i>Nominal flow rate case</i>	$\dot{m}_{in} = 15.54 \text{ kg/s}$ $T_{in} = 200^\circ\text{C}$
		<i>Low flow rate case</i>	$\dot{m}_{in} = 6.54 \text{ kg/s}$ $T_{in} = 200^\circ\text{C}$
	Outlet	$p_{out} = 0 \text{ Pa}$	
	Wire, cladding, blockage casing	No slip walls	$Q_{nom} = 197.66 \text{ kW}$
			$Q_{low} = 197.65 \text{ kW}$
	Hexagonal channel	Adiabatic no slip wall	

Table 4 – Simulations computational setup

The results for these two case scenarios are discussed in the next section, where the temperature distribution for the setup with the simultaneous presence of the small blockages will be displayed in comparison to the data from the experimental campaign. Subsequently, also the sensitivity analysis results will be explained, since they will be used as a reference for the CFD calculations obtained in this thesis. Once again, only the useful results in this framework will be presented for the sake of clarity, while for the complete analysis it is suggested to refer to the reference [46].

2.2.2 NRG CFD results and remarks

As it has already been done in the previous section regarding the experimental campaign results, the figures below show the comparison between the numerical and experimental temperature values retrieved at the thermocouples, that in the simulation are placed at the same location as in the test section. At one glance: the analyses done on the internal single sub-channel blockage setup show a reasonable prediction of the fluid temperature and pressure drop, in agreement also with the experiments performed in the analogous unblocked setup in the SEARCH project [58]. Indeed, the former mentioned results present a difference in the range of $\pm 10^\circ\text{C}$, while the bundle

⁷ The turbulent Prandtl number expresses the similarity between turbulent momentum exchange and turbulent heat transfer in a fluid. The turbulent part of the heat transport in low Pr number fluids is not so strongly coupled to the turbulent momentum transport, as it occurs for common fluids like water or air where it is possible to assume a constant ratio between turbulent heat transport and turbulent momentum transport, i.e. the Reynolds analogy. [57]

differential pressure is computed within 15% difference compared to the experiments. Nonetheless, the temperatures at the blockage interface are overpredicted up to 95°C.

Specifically, as far as the TCs at the blockages mid-height are considered, the outstanding result is that the temperatures are highly overestimated compared to the experiments, and even if they recover in the wake of the blockages, the discrepancy is around 20°C for C and 5-10°C for E1, as summarised in Table 5 and Figure 15.

TC letter	C1 related [°C]	E1 related [°C]
A	1.3	94.6
B	4.9	97.8
C	58.0	10.9
D	69.4	4.9
E (@ ML3 for E1)	62.7	-0.5
F	23.5	
G	18.0	
H (@ ML2 for C1)	17.7	

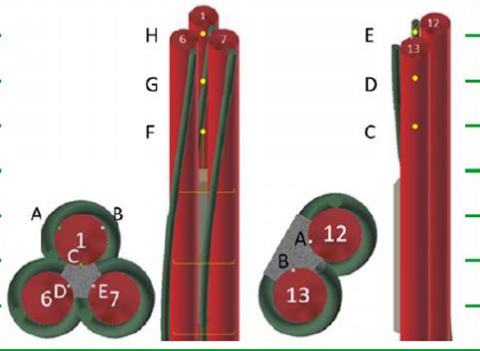


Table 5 – Difference between numerical and experimental temperature at the blockages mid-height and wake regions for the nominal flow rate case [46]

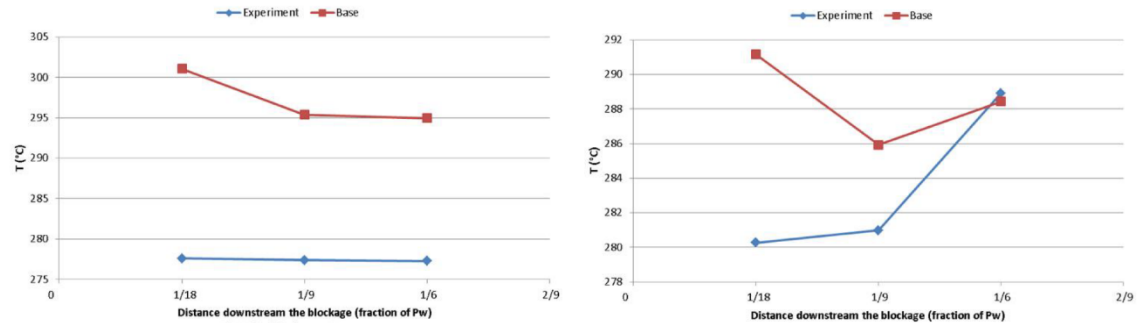


Figure 15 – Temperature distribution in C1 wake region (left) and E1 wake region (right): comparison between the NRG numerical results (red) and experimental data (blue) [46]

Further on, Figure 16 confirms that for both blockages the centre of the bundle is warmer than the side subchannels, in agreement with the experiments, yet the values obtained are different with their respect: temperatures are overestimated in the wake of the central blockage and underestimated in the side subchannels.

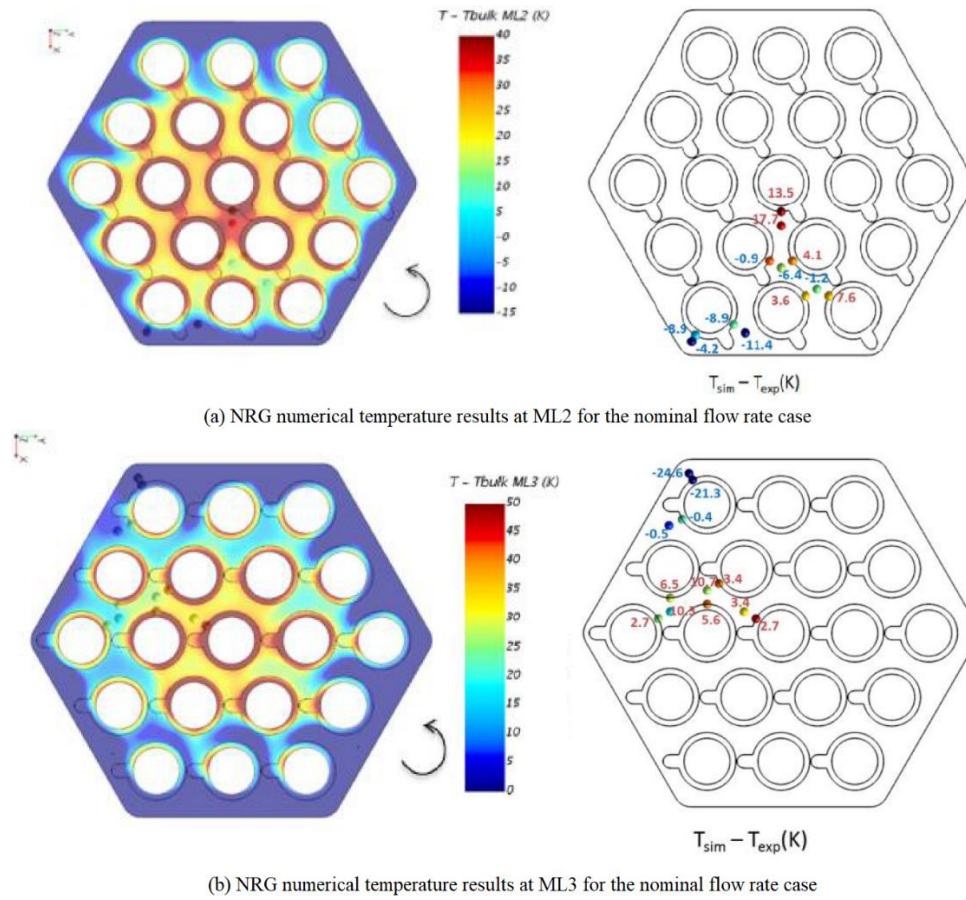


Figure 16 – Temperature distribution at the ML2 (a, left) and ML3 (b, left) and difference between numerical and experimental temperature values (right). The numerical bulk temperature is evaluated as mass flow average [46]

Considering the low flow rate case, the same conclusions as before can be drawn, yet the discrepancies are larger, since the power input is kept constant. For this reason, only the differences between the numerical and experimental values are reported below in Table 6 and Figure 17.

TC letter	C1 related [°C]	E1 related [°C]
A	12.7	86.4
B	16.0	96.0
C	69.7	8.7
D	67.5	12.0
E (@ ML3 for E1)	69.7	-0.3
F	33.0	
G	29.8	
H (@ ML2 for C1)	30.2	

Figure 17 is a schematic diagram of the NRG blockages. It shows a central vertical column of blockages with points A, B, C, D, E, F, G, and H marked along its length. To the left of this column are two circular blockages labeled 1, 2, 3, 4, 5, 6, 7, and 8. To the right of the central column are two circular blockages labeled 12 and 13. The diagram illustrates the spatial arrangement of the blockages and the locations of the temperature measurement points.

Table 6 – Difference between numerical and experimental temperature at the blockages mid-height and wake regions for the low flow rate case [46]

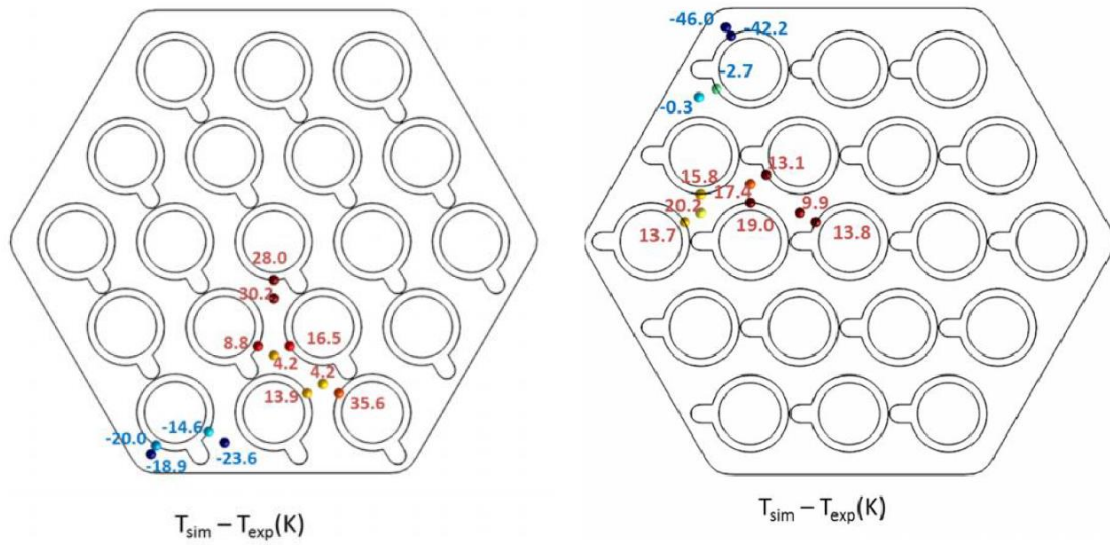


Figure 17 – Difference between numerical and experimental temperature at ML2 (left) ML3 (right) for the low flow rate case [46]

2.2.3 Sensitivity analysis

In order to explain the big discrepancy in the numerical results compared to the experimental data, a series of sensitivity studies is performed on the low flow rate case scenario, but unfortunately they show small sensitivity to most of the modelling parameters, like mesh density, change in thermo-couple position of 0.1 mm, variation the turbulent Prandtl number, change the turbulence formulation and inclusion of conjugate heat transfer in the hexagonal channel. On the contrary, a larger impact is seen with leakage paths between blockages and fuel pins, i.e. LBE flows in potential gaps present, and with an increased thermal conductivity of the blockage, resulting in a higher decrease in the temperature values, yet effect quickly disappearing downstream.

Firstly, as far as the mesh refinement is concerned, a wall resolved mesh has been implemented, leading to a big increase in the number of cells (69.2 million, 63.7 million of which in the fluid only) and consequently a big decrease in the y^+ value (an average of 0.8 for the rods and wires, and 0.7 for the hexagonal channel). As already mentioned, the small impact of the mesh sensitivity on the temperature in the major part of the domain (4.6°C maximum difference at ML2 and 9.4°C at ML3) doesn't explain the discrepancy in the numerical and experimental values, therefore the accuracy gained with the mesh refinement doesn't justify the additional computational cost.

Secondly, the possible uncertainty in the thermocouple position has been investigated, due to their small dimension and high technical precision required. For this reason, the potential variation of

the temperature value with the location has been evaluated changing the position of the numerical probe of 0.1mm from the original design. Anyway, the sensitivity showed is marginal: at most 1.5°C difference for subchannel TCs and 3.2°C for the ones near the blockages.

Moreover, the Turbulent Prandtl number, parameter which takes into account that the hydraulic and thermal boundary layer thickness are different for the heat transfer modelling of liquid metals (oppositely to water and air), has been varied as well: its decrease to 1.5 showed a change lower than 0.7°C and its increase to 4.0 resulted in a maximum difference of 1.45°C. Thus, the gap with respect to experimental data cannot be ascribed to this parameter either.

Totally equivalent conclusion can be drawn from the sensitivity study on the formulation of the turbulence model and the inclusion of the conjugate heat transfer in the hexagonal channel. Indeed, the former resulted in a change of at most 2°C, whereas the latter showed a difference of about 0.1°C for the TCs related to C1 and at most of 4.2°C for the ones related to E1. In fact, evidence [59] explain that allowing conductive heat transfer in the hexagonal steel channel affects the distribution of the temperature in the outer subchannels, therefore the impact on the edge blockage is larger, because cooling by conduction is present.

On the other hand, more interesting findings are obtained by the postulated presence of leakage paths between the rods and the blockages, and by changing the thermal conductivity of the blockage material. As far as the first study is concerned, it has been already mentioned that such leakages could be eventually present due to construction uncertainties in the test section (the small blockages are welded only on the top and bottom). Hence, they are modelled in the CFD simulations by replacing the steel shell of the blockages with liquid LBE. Although this modification resulted in a quite big temperature decrease downstream E1 (more than 10°C) because relatively cold LBE can flow in the gap with the external channel, for the wake region of C1 is not the case. Nevertheless, the striking results are found in at the blockages: at C1 the decrease is in the range of 10-40°C depending on the TC, and over 100°C at E1. In conclusion, the thermal conductivity of the filling ceramic paste has been increased, since the properties have been given by the provider and might be affected by uncertainty. The biggest impact is observed at the TCs near the blockages: a decrease of about 10°C is seen at C1 and about 20°C at E1, but it is smaller than 0.25°C at the other TCs. It is important to mention at this stage that the model showed a big sensitivity to these two last mentioned studies, yet only for the TCs at the interface with the solid blockages, resulting instead to a little effect in the prediction of the other temperatures.

In the chapters that follow, the detailed description of the process, with which the CFD model of this thesis has been built, will be given. The obtained results for all cases analysed are compared both to the NRG numerical results and to the experimental data retrieved at the KIT-KALLA test section, in order also to prove the reliability of such model. In addition to the main aim of the thesis, which is the investigation of the effect of the presence of heat-emitting porous blockages in the hexagonal channel 19-pin wire-wrapped fuel bundle previously described, additional studies have been done in order to understand better the reasons lying beneath the discrepancy found in the numerical and experimental results

Chapter 3 – Fuel assembly model without blockage

Starting from the present chapter on, the explanation of the procedure with which the CFD models used in this thesis have been developed is given. A structured step-by-step methodology has been implemented, starting from a simplified base model, where only the working fluid domain has been modelled, and gradually adding specifications, like the rod claddings and wires and the blockages. Accordingly, the modifications to the models have been made and different approaches have been analysed in order to find the best one representing the phenomena involved.

The results obtained from this preliminary approach to the modelling of the 19-pin wire-wrapped fuel bundle are compared to the corresponding experimental data deriving from the experimental campaign within the European project SEARCH at KIT-KALLA where the tests have been performed on an unblocked test section. [58]

3.1 Flow description

As suggested by the title, in this chapter the model for the unblocked scenario of the 19-pin wire-wrapped fuel bundle is described, in order to start to investigate and understand the behaviour of the liquid LBE inside the channel. As previously mentioned, a progressively more detailed setup has been built, which explains the rationale according to which the unblocked scenario has been investigated. Besides, an investigation of different approaches has been done: at first, only the fluid domain has been modelled, applying a uniform distributed power at the surface corresponding to the outer diameter of cladding and imposing an adiabatic wall boundary condition at the surface corresponding to the wires. These stringent conditions were not fully representing the occurring physical phenomena, therefore it has been necessary to add the claddings and the wires, and accordingly to apply the power at the inside of the steel cladding. This modification allows the heat transfer between the interfaces, since the wires have the dual purpose of keeping the fuel pins in place, guaranteeing the appropriate distance, and of acting as turbulence promoters and heat exchanging fins. In addition, it is important to mention that two different approaches have been used for the specification of the inlet boundary condition: initially, an inlet mass flow rate condition has been set, corresponding to a uniform inlet velocity profile. Subsequently, by the implementation of periodic boundary conditions⁸, it has been possible to set a fully developed velocity profile,

⁸ Periodic boundary conditions are often chosen for approximating a large numerical system by using a smaller section, i.e. unit cell, and in the case the geometry and the expected flow pattern have a periodically repeating nature, that is the flow across two opposite planes in the computational model are identical. Periodic boundary conditions can be applied to a pair of boundary sections, and at such inlet and outlet the

condition that allowed to obtain a more representative fluid flow condition at the beginning of the heated section, compared to a uniform hydraulic field. Besides, a faster convergence of the code and to lower its computational cost are achieved, since a shorter domain could be used to obtain a developed flow. For these reasons, only the more realistic case will be discussed in detail.

3.1.1 Geometry

The geometry of interest is the 19-pin wire-wrapped fuel bundle embedded in an hexagonal channel used in the THEADES loop at KIT-KALLA, extensively described in the section “2.1 Experimental background”, and dimensions of which are specified in Table 15. As represented in Figure 18, the initial choice has been to limit the domain to a length of one wire pitch, in order to limit the computational cost, yet still capturing the main occurring phenomena. The liquid LBE upward flow follows the positive direction of the z-axis.

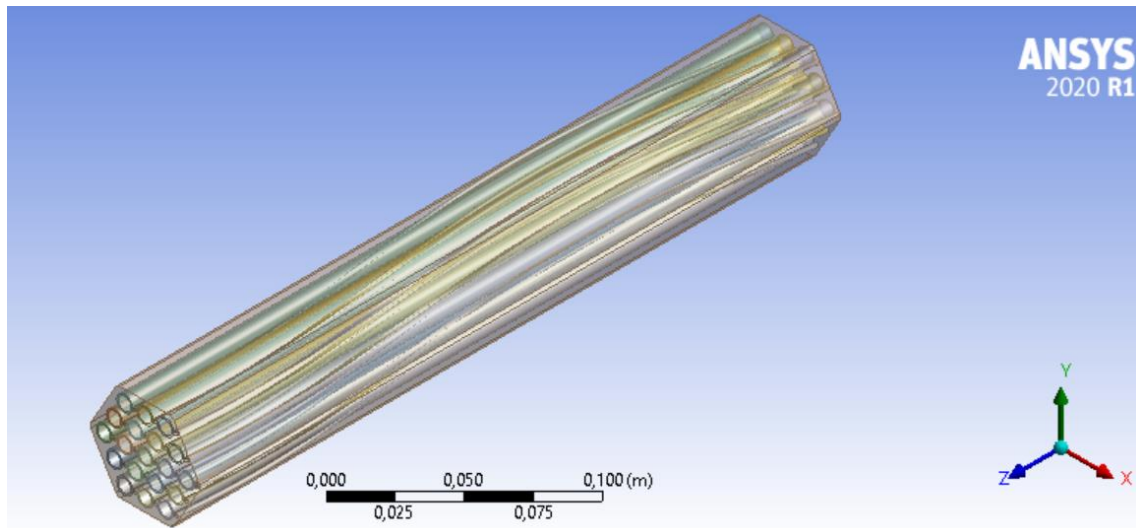


Figure 18 – Computational domain of the unblocked case scenario

The other investigated option is equivalent to the previous one but extended to three pitch long domain. This configuration has been modelled in order to have a closer correspondence to the experimental test section, therefore used also to spot eventual numerical discrepancies with the model with separated domains. Nevertheless, it is clear that given the bigger dimension, the number of cells had to be limited to a reasonable quantity not to increase excessively the computational cost of the simulation. Hence, the above-mentioned geometry has been preferred,

velocity profile for the inlet and outlet will be the same, yet a difference of normal force or pressure will be allowed between them. [60]

due to the gain in numerical accuracy (more refined mesh given the same domain extension) and the computational time (smaller domain).

3.1.2 Materials and working fluid

The working fluid is the liquid metal LBE, whose thermophysical properties are taken from [26], as described in the paragraph “1.4 Lead-Bismuth Eutectic as nuclear coolant”. The solid structures, namely the cladding and the wire of the fuel pins are instead made in stainless steel [61]. The temperature dependent empirical correlations, which are implemented in the code, are listed in Table 7.

	LBE	Stainless steel DIN 1.4571
Density [kg/m³]	$\rho(T) = 11096 - 1.3236 * T$	$\rho(T) = 8040.3 - 0.44165 * T + 2.071 * 10^{-5} * T^2 - 5.8048 * 10^{-8} * T^3$
Specific heat [J/kg K]	$c_p(T) = 159 - 2.72 * 10^{-2} * T + 7.12 * 10^{-6} * T^2$	$c_p(T) = 456.2817 + 0.4337 * T - 5.7714 * 10^{-4} * T^2 + 3.5074 * 10^{-7} * T^3$
Thermal conductivity [W/m K]	$\lambda(T) = 3.61 * 1.517 * 10^{-2} * T - 1.741 * 10^{-6} * T^2$	$\lambda(T) = 13.28571 + 1.756205 * 10^{-2} * T - 5.378788 * 10^{-6} * T^2 + 4.292929 * 10^{-9} * T^3$
Viscosity [kg/m s]	$\mu(T) = 4.94 * 10^{-4} * \exp\left(\frac{754.1}{T}\right)$	–

Table 7 – Temperature dependent thermophysical properties of LBE [26] and stainless-steel DIN 1.4571 [61]

3.1.3 Assumptions

The assumptions made in order to carry out the computational fluid-dynamic analysis are the following:

- Turbulent LBE flow, under steady state condition;
- Incompressible flow;
- Temperature dependant fluid and solid physical properties;
- Fluid entering the channel with fully developed velocity profile and uniform temperature. In specific, it is assumed that the velocity boundary layer is fully developed, hence the thermal one starts developing and due to the low Pr number typical of liquid metals, the large role played by molecular thermal diffusivity is comparable to the turbulent diffusivity, resulting in a relatively thick thermal boundary layer [62];
- Constant heat flux at the internal cladding surfaces, negligible gravitational force, even if the channel is vertical and Turbulent Prandtl number equal to 0.9. These three hypotheses will be relaxed and investigated later in this text.

3.2 Simulation setup

In order to understand whether the model developed was properly predicting the flow phenomena, the setup of the model described in the present section represents the reference unblocked scenario of the wire-wrapped 19-pin hexagonal rod bundle that has been investigated in the experimental campaign within the European project SEARCH at KIT-KALLA. [58]

3.2.1 Computational domain

The computational domain is based on the geometry described in the paragraph above (see “3.1.1 Geometry”) and in order to achieve a better accuracy and prediction of the results, as well as a faster convergence of the model, it constitutes of two separated simulations, in which a first unheated wire pitch long domain is used for the hydraulic flow development, whose velocity profile is then given as inlet condition to a domain alike where the heating is imposed (Figure 19). It is important to mention that in the isothermal simulation destined to the hydraulic field flow development only the fluid domain has been modelled, since the absence of heat transfer allows to neglect the solid part.

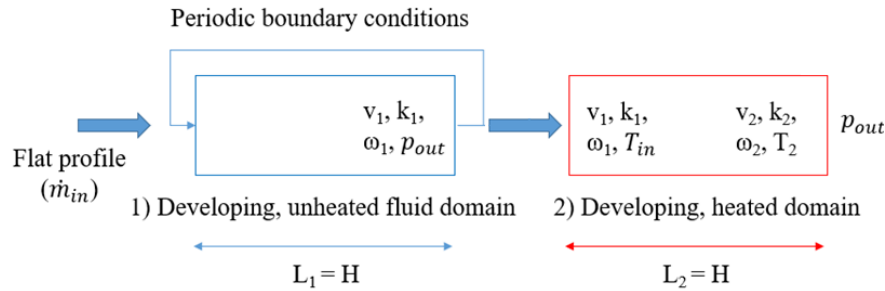


Figure 19 – Sketch of the computational domain of the unblocked case scenario

3.2.2 Boundary conditions

The fluid operating conditions imposed in this model are the ones representing the design of the MYRRHA reactor and are summarised in Table 8.

Domain	Surface	Boundary condition
Fluid (LBE)	Hexagonal channel	No slip condition, adiabatic walls
	Inlet	$\dot{m}_{in} = 19.18 \text{ kg/s}$ $T_{in} = 200^\circ\text{C}$
	Outlet	$p_{out} = 0 \text{ Pa}$
Solid (SS 1.4571)	Internal rod surface	$q'' = 0.578 \text{ MW/m}^2$
Interface	Wires and external cladding surface	Conservative interface flux

Table 8 – Reference case boundary conditions specification

It is important to clarify that the inlet conditions of the heated domain under investigation are imposed as fully developed velocity profile with related turbulence parameters, retrieved by the isothermal with periodic boundary conditions simulation, and uniform inlet temperature. The heat flux (q'') is uniformly distributed on the internal surfaces of the rod cladding, and it is evaluated by the power specification (Q) with Equation 2, where N is the number of rods, R_{int} is the cladding inner radius and L_{heat} is the heated length and whose values are in Table 15:

$$q'' = \frac{Q}{N 2\pi R_{int} L_{heat}} \quad (2)$$

3.2.3 Models

The physics models of the simulation are set as following:

- *Space*: Three dimensional. This is clearly because it is not possible to reduce further the dimension of the problem, since none of the directions can be neglected and there is no symmetry to be exploited;
- *Time*: Steady. The choice of this solver is done because the flow is macroscopically steady, with no specific driver of transient flow, i.e. the mass flow rate is always constant. This selected time solver is thus cheaper under a computational point of view;
- *Material*: LBE. The single-phase fluid chosen is LBE, whose properties are temperature dependant and specified in section “3.1.2 Materials and working fluid”;
- *Flow*: Coupled flow. The code uses a coupled solver, which solved the hydrodynamic equations (one per each velocity component and one for the pressure) as a single system. The approach implemented uses then a fully implicit discretization of the equations at any given time step. Additionally, as in this case of a steady-state problem, the time-step is considered to be an “acceleration parameter”, that guides the approximate solutions in a physically based manner to a steady-state solution. The number of iterations required to reach convergence is therefore reduced; [60]
- *Viscous regime*: Turbulent;
- *Turbulence model*: SST k- ω Turbulence (RANS). A more detailed description of the theory behind the turbulence modelling can be found in “Appendix B – Numerical modelling theory”;
- *Energy model*: Thermal energy. This model solves the energy equation, therefore modelling the transport of enthalpy through the fluid and it is suitable for heat transfer in low-speed flows, where variable-density effects are negligible. [60]

It must be specified that due to the complexity of the concerning numerical simulation of flow and thermal field, it is still unclear which should be the best performing turbulence model for this specific geometry. Indeed, the swirling effect given by the wire presence and eventual recirculation and flow detachment in their wake, along with an imposed heat flux condition at the wall, are representing a challenge for every RANS model. Based on the literature review done [63] [64] [65], the choice done has been to start the analysis applying the SST $k-\omega$ model, because it addresses some specifics flaws of the standard model (see section “B.1.2 $k-\omega$ model”), like the sensitivity to free-stream turbulence levels, and it can be applied to the viscous affected region without further modifications. Additionally, it accurately predicts both of the viscous sublayer and core region of wall bounded internal flows.

3.3 Mesh generation

It is clear that in order to mesh properly the domain it is necessary to apply both a surface and a core mesher. Indeed, to have a well-structured mesh at the wall, i.e. where the major gradients are present, an inflation layers should be used, in order to fix and control the y^+ of the mesh, to model with sufficient accuracy the viscous sublayer at the walls. Yet, at this preliminary stage of the analysis the structured layer of prisms at the walls of the hexagonal channel and rods haven't been imposed and the generated mesh, with approximately 5.7 million tetrahedral cells, 3.7 million of which are in the fluid domain, is displayed below in Figure 20.

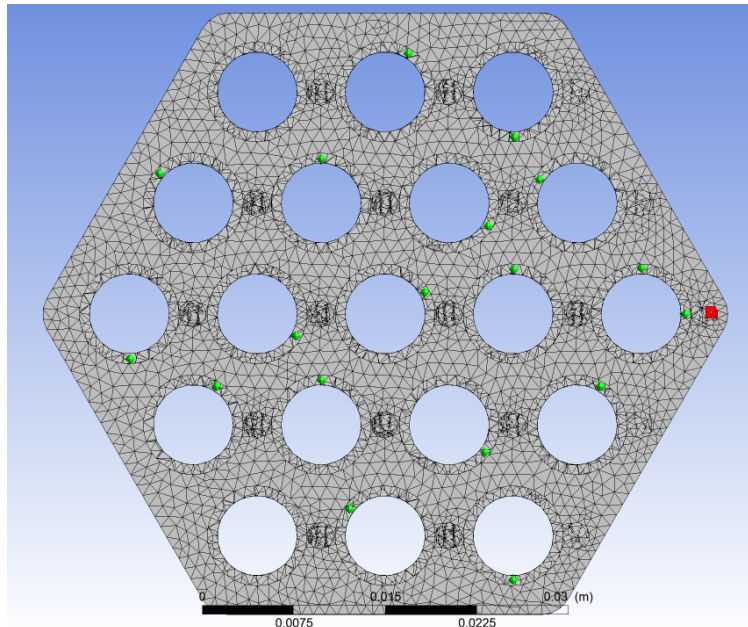


Figure 20 – Mesh of the cross-section of the 19-pin wire-wrapped fuel bundle of the unblocked reference case

3.4 Results

In this paragraph the preliminary results for the unblocked section case scenario will be presented. As already explained in “Chapter 2 – ”, the values are taken at the TCs installed at the measurement plane (Figure 21), which is located at 54.6 mm downstream the onset of the heating, as represented in Figure 22. The green dots in the figure below are representing the TC embedded in the cladding of the fuel pins, while the red squares are the ones which are hanging in the bulk of the fluid subchannels. The numerical results are reported in comparison to the experimental data, which is affected by an uncertainty of ± 0.10 K.

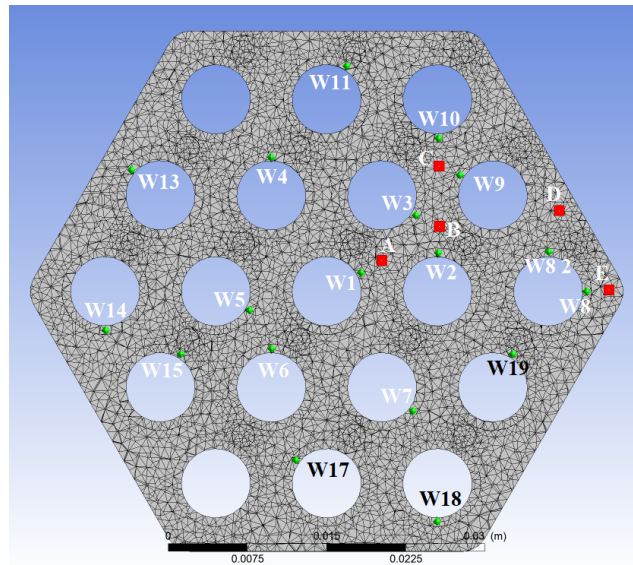


Figure 21 – Representation of the TC position at ML1

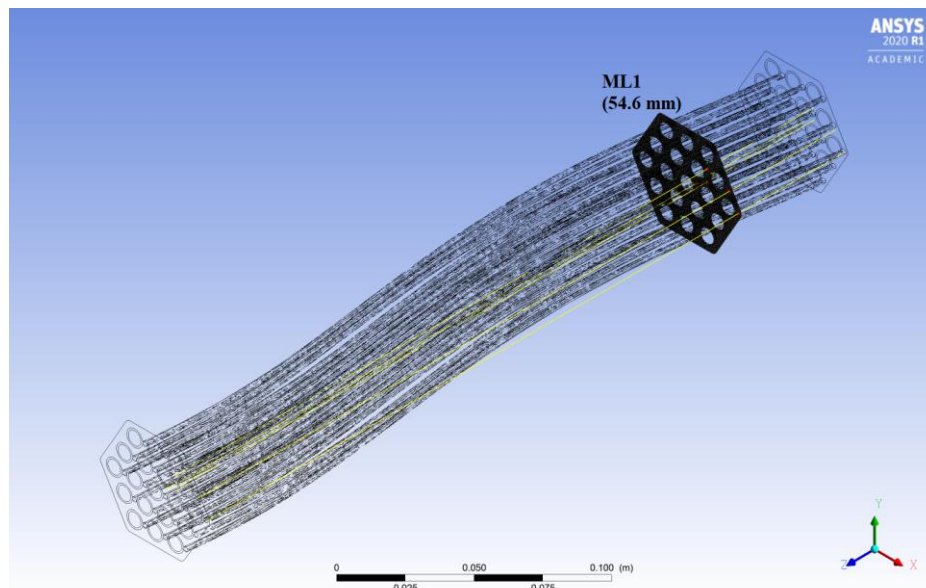


Figure 22 – Representation of the position of ML1

The results retrieved at such respective TCs are separated by a black vertical line in Figure 23: the values at its left are the temperatures measures in the claddings, whereas on its right are the measurement of the fluid temperature. The grey horizontal line represents the bulk temperature at the location of the ML1, evaluated with an energy balance equation.

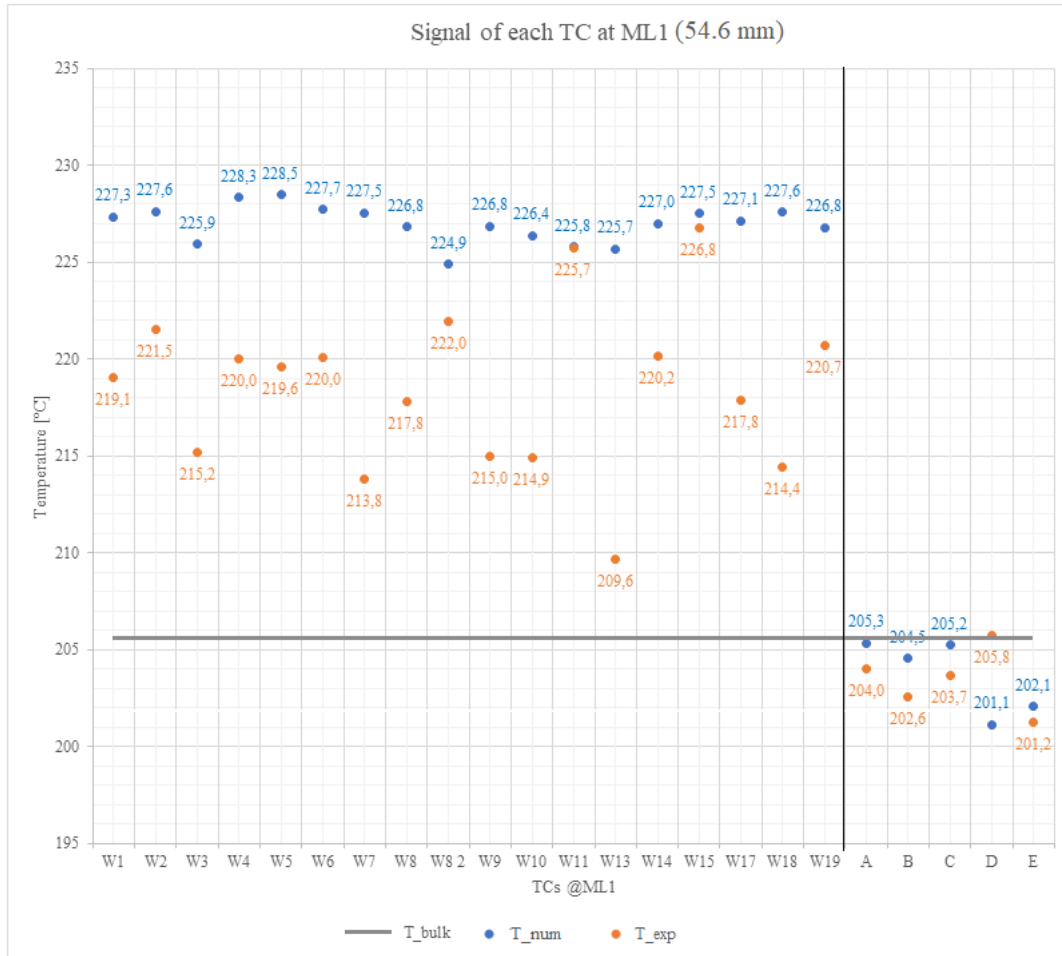


Figure 23 – Comparison of the temperature between the numerical and the experimental values at the TCs placed at ML1

It is clear that there is a general overprediction of the temperatures at every position, much more pronounced at the location inside the fuel pins claddings. The much closer difference in values obtained in the fluid subchannel, at most of 2°C, allows to conclude that the differences observed are due to the poor resolution of the near-wall region, since for the preliminary assessment of the model the inflation layer has not been inserted, resulting in a value of y^+ about 97.1 at the surface close to the fuel rod cladding and wire and 122.7 at the hexagonal channel walls.

In Figure 24 are shown the lines passing through the points at which the TCs in the bulk of the subchannel are placed. Along these lines the temperature distribution has been retrieved and it is depicted in Figure 25.

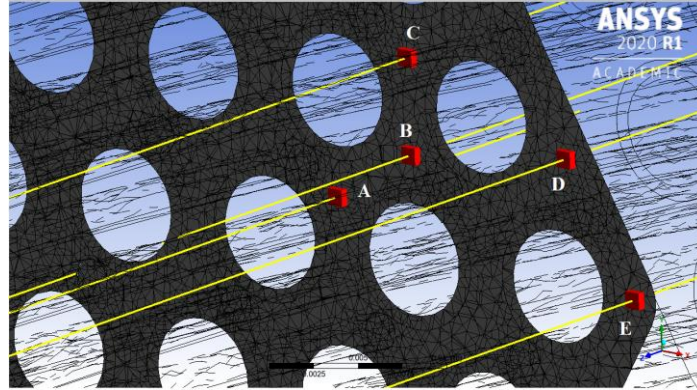


Figure 24 – Representation of the sampling lines for the axial temperature profiles

From the plot below it can be seen how the temperature in the more central part of the fuel is warmer (along the sampling lines corresponding to the TC “A”, “B” and “C”) , compared to the region at the boundary close to the hexagonal channel (along the sampling lines corresponding to the TC “D” and “E”), which is explained by the lower heating of this region (the hexagonal wall is not heated) and the higher velocities in the corners, due to the narrower subchannels. In all cases it warms up quickly, starting from the uniform inlet temperature imposed. The jumps that are visible are corresponding to where the line is crossed by the helicoidal wire, therefore the recorded temperature is higher.

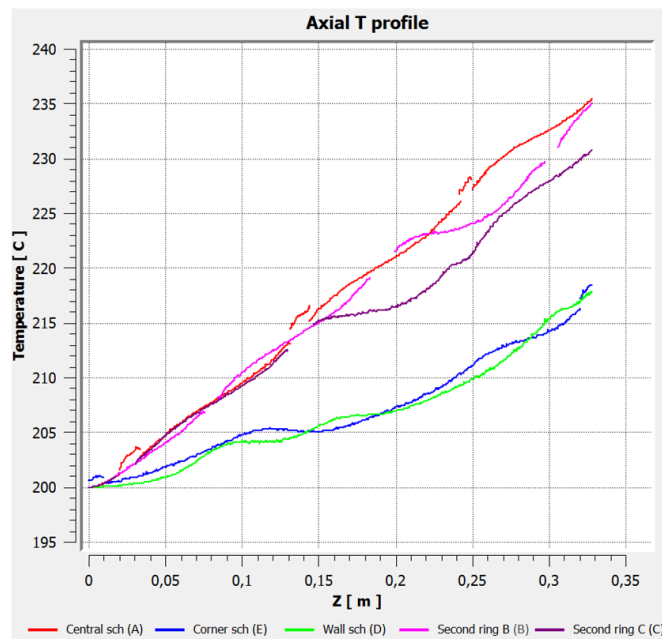


Figure 25 – Temperature profile along the axial direction (the letters between brackets are the corresponding TC)

The abovementioned trend is also demonstrated in Figure 26, which is depicting the temperature contour plot at ML1. As expected, the hottest spots are found in the region where the contact between the wire and rods is located, and instead the bulk fluid in the subchannel is always colder. Additionally, the more or less homogeneous temperature in the fluid over the ML1 suggests that the plane is located relatively close to the onset of the heated length, and therefore the heat transfer from the fuel pins to the bulk fluid is not yet complete.

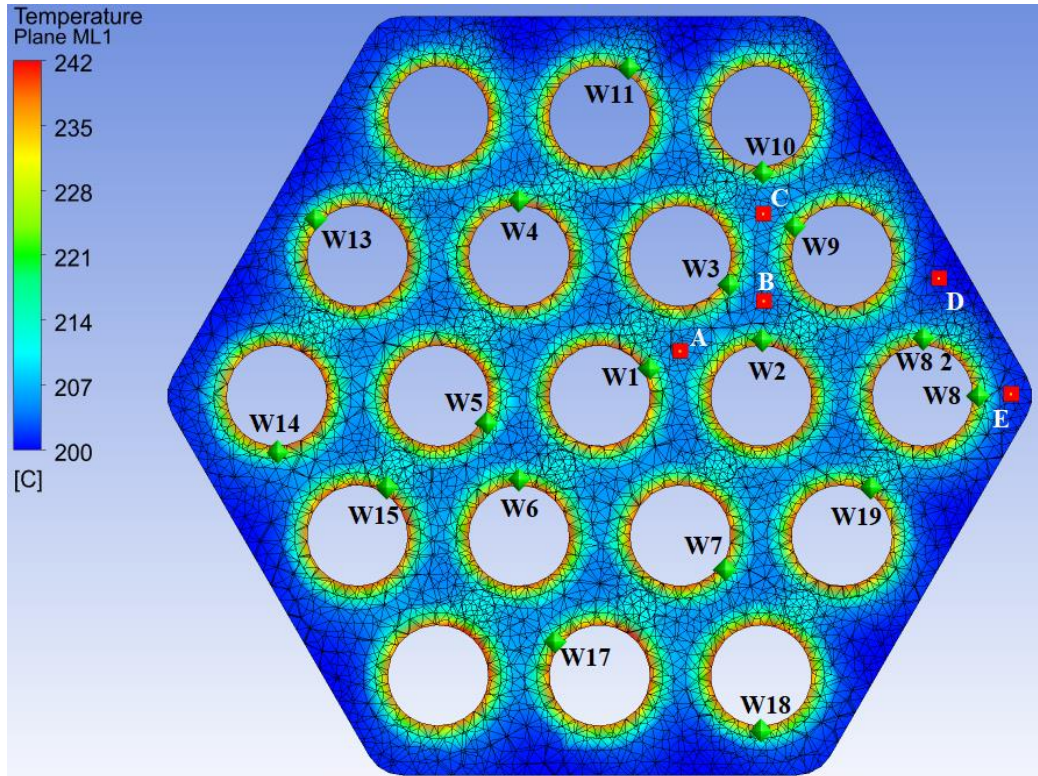


Figure 26 – Temperature contour plot at the ML1 for the unblocked case scenario

It is important to specify that however the accordance of the results of the unblocked domain section with the experimental data of the SEARCH campaign have been verified after the appropriate modifications to the model have been applied. The specific characteristics of the model, as well as the results, are explained in “Chapter 4 – Fuel assembly model with solid blockage”.

At this stage of the discussion is then relevant to anticipate that solving the issues related to the appropriateness of the domain in terms of mesh and problem resolution in the near-wall region gives a big contribution in the prediction of the temperatures, since the difference in the values has been significantly decreased.

Given the more promising results, suggesting the good accordance with the general behaviour of the flow inside the fuel bundle, as well as a better prediction of the values of the temperatures at every TCs, it has been decided to proceed with the analysis, modifying once more the model in order to include the obstruction of one of the central subchannels by a solid blockage, as it has been done in the experimental campaign described in section “2.1 Experimental background”. [45]

3.5 Conclusions

In the chapter here above discussed, the unblocked case scenario of the 19-pin wire-wrapped fuel bundle have been discussed as preliminary assessment of the modelling of the geometry under investigation. The procedure used has been explained, presenting the details of the assumptions made, the geometry and mesh used, as well as the computational setup has been described.

The results obtained from this preliminary approach to the modelling of the 19-pin wire-wrapped fuel bundle are compared to the corresponding experimental data deriving from the experimental campaign within the European project SEARCH at KIT-KALLA where the tests have been performed on an unblocked test section. These, although initially discouraging due to a big difference encountered in the prediction of the temperatures, mostly at the locations where the TCs are placed in the rods’ cladding, in comparison with the experimental data, have later shown a good accordance with the values obtained in the tests, and therefore it has been decided to proceed with the analysis and with the implementation of a solid blockage obstructing a central subchannel. This case scenario will be discussed in “Chapter 4 – Fuel assembly model with solid blockage”.

Chapter 4 – Fuel assembly model with solid blockage

Given the fact that partial subchannel blockage has been considered to be a probable occurring event in off-normal conditions, in order to support the development of the safety assessment of liquid metal cooled reactor systems the present chapter will exemplify the procedure with which the CFD model of the 19-pin fuel bundle comprising solid blockages has been developed.

As mentioned already for “Chapter 3 – Fuel assembly model without blockage”, a similar progressive approach has been used: firstly, only the central blockage element was added to the fluid domain, applying the uniform distributed power at the surface corresponding to the outer diameter of cladding and imposing an adiabatic wall boundary condition at the surface corresponding to the wires. Once again, such conditions weren’t representing the real phenomena, therefore it has been necessary to add the claddings and the wires, in order to allow the heat transfer between the interfaces. For the same reasoning as before, only the second realistic case will be discussed. It is important to mention that the choice of modelling only the central blockage (thus not the edge blockage) has been taken because by shortening the domain it has been possible to increase the number of cells and therefore decrease the computational time. Additionally, based on the previous work done by NRG [46], it has been proved that there is no mutual influence of the blockages.

4.1 Base case geometry modification and materials

The geometry used in this model is the same that has been implemented in the previous chapter (section “3.1.1 Geometry”), with the only difference that the central blockage has been added adjacent to the central pin, blocking one of the central subchannels, exactly corresponding to how it has been implemented in the test section mentioned above (section “2.1.2 Description of blocked setup”).

As far as the materials are concerned, they are the same used both in the experimental campaign and in the prior numerical simulation, which specifics can be found in “Appendix A – Detailed description of the background experimental campaign and numerical simulation”.

4.2 Blocked reference case

4.2.1 Computational domain

The computational domain has been built following the same procedure and rationale used in the previous chapter, with the addition of a third separated simulation containing the central blockage. For the sake of clarity, the domain visible in Figure 27 is composed in specific by:

1. A first one wire pitch (H) long unheated domain, unblocked and composed only by fluid domain, in which the velocity and pressure profiles development through periodic BCs implementation is achieved;
2. A second one wire pitch long heated domain, unblocked and where conjugated heat transfer is allowed with the claddings and wires. Here the hydraulic field established previously is imposed as BCs, and the temperature profile is developing;
3. Finally, the blocked section is modelled, longer than one wire pitch in order to avoid the influence of the outlet boundary conditions on the results, which is the same reason behind the imposition on an outlet pressure profile, instead of a uniform outlet pressure boundary condition.

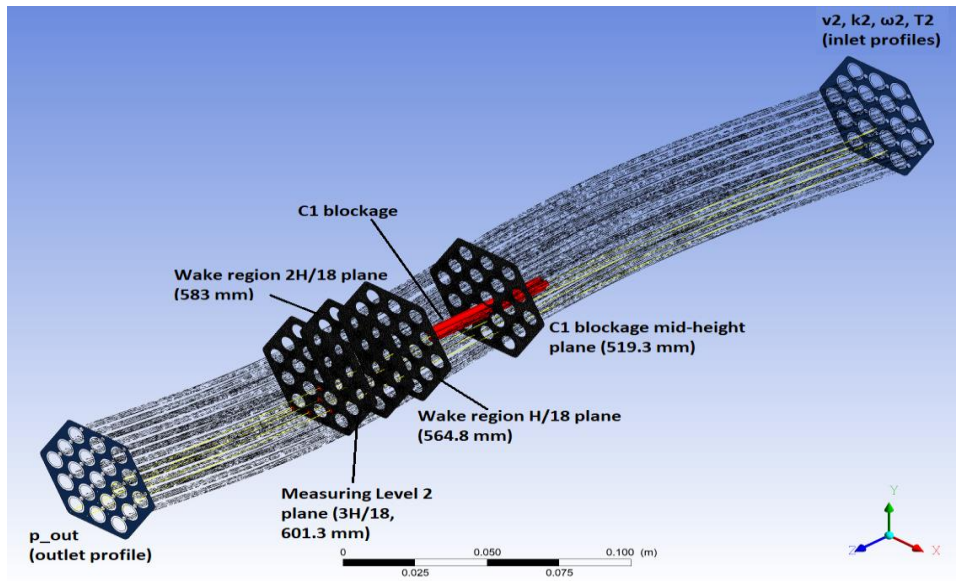
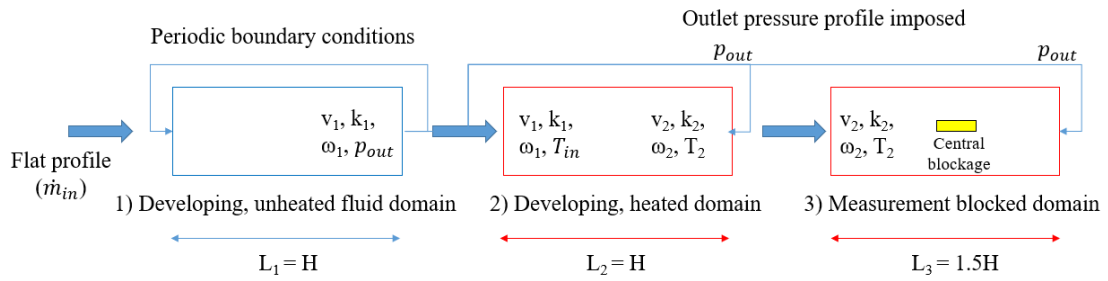


Figure 27 – Computational domain with boundary condition specification: sketch of the complete domain (above), blocked domain with specification of the measuring levels (below)

4.2.2 Setup

The fluid operating conditions imposed in this model are corresponding to the nominal MYRRHA reactor ones, as far as heat flux and Reynolds number are concerned. The computational setup is visible in Table 9, where the assumptions and the rationale have been already explained in the previous chapter.

Methods	SST k- ω Turbulence (RANS), Turbulent Pr = 0.9	
Time dependence	Steady state	
Domain	Surface	Boundary condition
Fluid (LBE)	Hexagonal channel	No slip condition, adiabatic walls
	Inlet	$\dot{m}_{in} = 15.54 \text{ kg/s}$ $T_{in} = 200^\circ\text{C}$
	Outlet	p_{out}
Solid (SS 1.4571)	Internal rod surface	$q'' = 0.580 \text{ MW/m}^2$
	Wires and external cladding surface	Conservative interface flux with LBE and blockage
Central blockage	Paste and shell	Conservative interface flux with LBE, claddings and wires

Table 9 – Blocked reference case boundary conditions specification

As already mentioned in the previous paragraph, the inlet conditions of the both blocked and unblocked heated domains are imposed as fully developed velocity profile with related turbulence parameters, retrieved by the isothermal with periodic boundary conditions simulation. From this simulation also the outlet pressure profile has been retrieved and imposed as outlet boundary condition for both the successive sections, in order not to influence the results. In the same fashion, the temperature inlet condition is at first imposed as uniform for the unblocked domain and subsequently the developed temperature profile is imposed to the blocked section inlet boundary. Once again, the heat flux (q'') is uniformly distributed on the internal surfaces of the rod cladding.

4.2.3 Mesh generation

Accordingly to what has been said in the previous chapter (see section “3.3 Mesh generation”), in this case an inflation layer of prismatic cells has been added for the wall treatment, necessary to capture with sufficient accuracy the viscous phenomena occurring at the walls. Although as explained in section “B.2 Wall treatment” the model requires a fine mesh with near wall cells $y^+ \sim 1$ in order to solve the viscous sublayer, due to also the demanding numerical characteristics

of the chosen turbulence model, with the initially used mesh and simulation setup a higher value is reached. Nevertheless, it is important to mention that even exploring other turbulence models and refining the mesh, in order to reach a more appropriate and consistent application of the solvers, the accuracy of the solution is not improved as expected.

In the simulation of interest the generated mesh shown in Figure 28 presents a structured inflation layer around the wire, cladding and hexagonal channel region, in order to capture the phenomena in the near-wall region, whereas an unstructured grid of tetrahedrons has been created in the fluid domain.

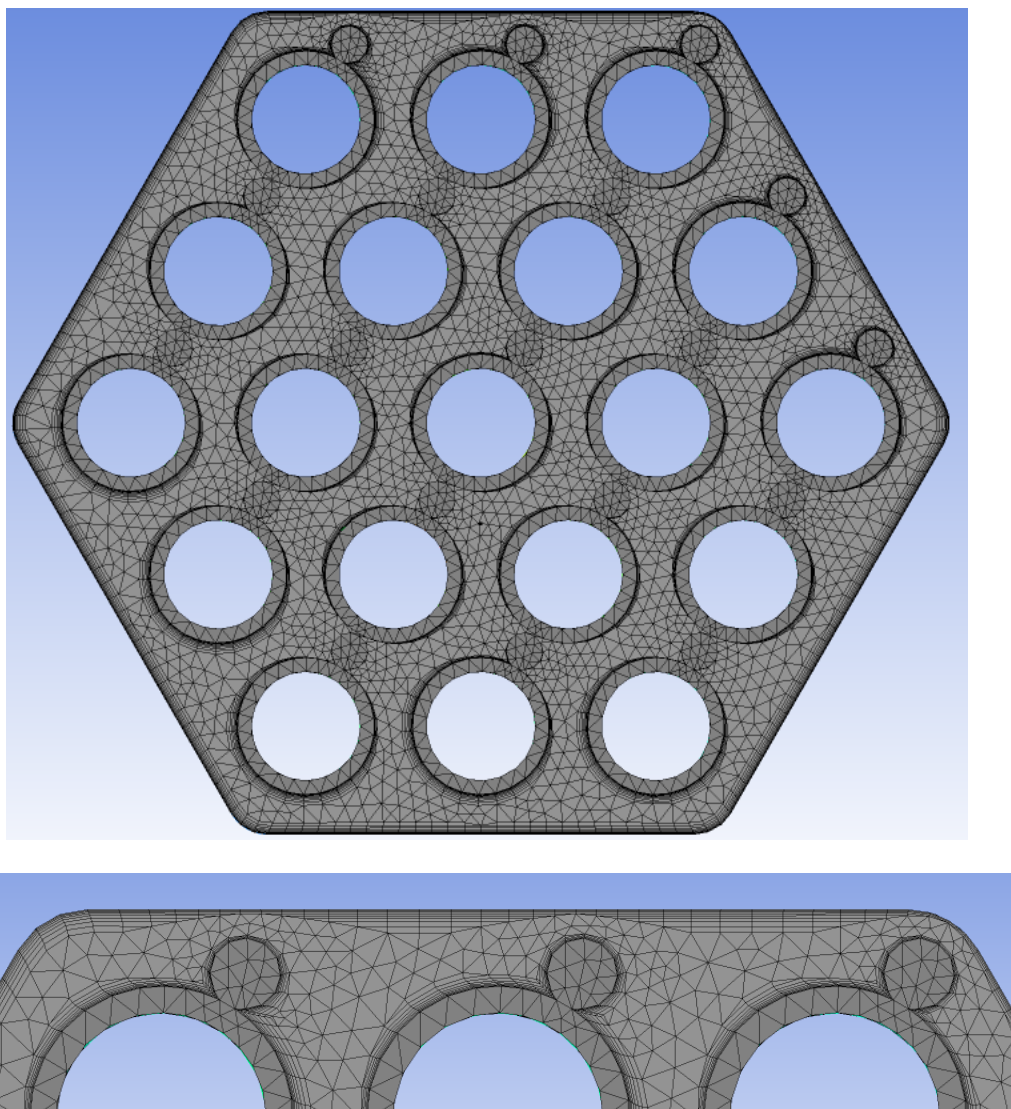


Figure 28 – Mesh of the 19-pin wire-wrapped fuel bundle of the base reference case: whole cross-section at the outlet (above) and close-up of the top portion (below)

As summarised in the specifics (Table 10), the inflation layer settings are such to cover as much as possible the boundary layer thickness, therefore several layers of prism cells with increasing thickness per layer in the radial direction are defined, in order to have also a smooth transition with the first cells present in the bulk of the domain and avoid big discrepancies in the results.

1st layer cell height	3e-5 m
Maximum N# layers	8
Growth rate	1.3
Total N# cells	14.9e6
N# cells in fluid (LBE)	10.8e6
N# cells in cladding and wire	4e6
N# cells in blockage	41.8e3 (paste) 22.6e3 (shell)
Avg y+ at cladding and wire walls	10.47
Avg y+ at hexagonal channel walls	12.46

Table 10 – Specifics of the generated mesh

4.2.4 Results

First of all, it is of relevant importance to specify at this stage of the discussion that an additional check has been done on the unblocked domain section to verify the accordance with the experimental data of the SEARCH campaign. The specific characteristics of the model are the ones explained in this chapter and the results are visible in Figure 29, where the temperature values are sampled at the same TCs location of Figure 21. The results here below reported are compared to the experimental data, which is affected by an uncertainty of ± 0.10 K.

It is clear that solving the issue of the appropriateness of the domain in terms of mesh and problem resolution in the near-wall region discussed in section “3.4 Results” gives a big contribution in the prediction of the temperatures, since the difference in the values has been significantly decreased. Indeed, the discrepancy encountered is in the range of 6K at the location of the TCs inside the cladding, and even lower in the ones in the subchannels.

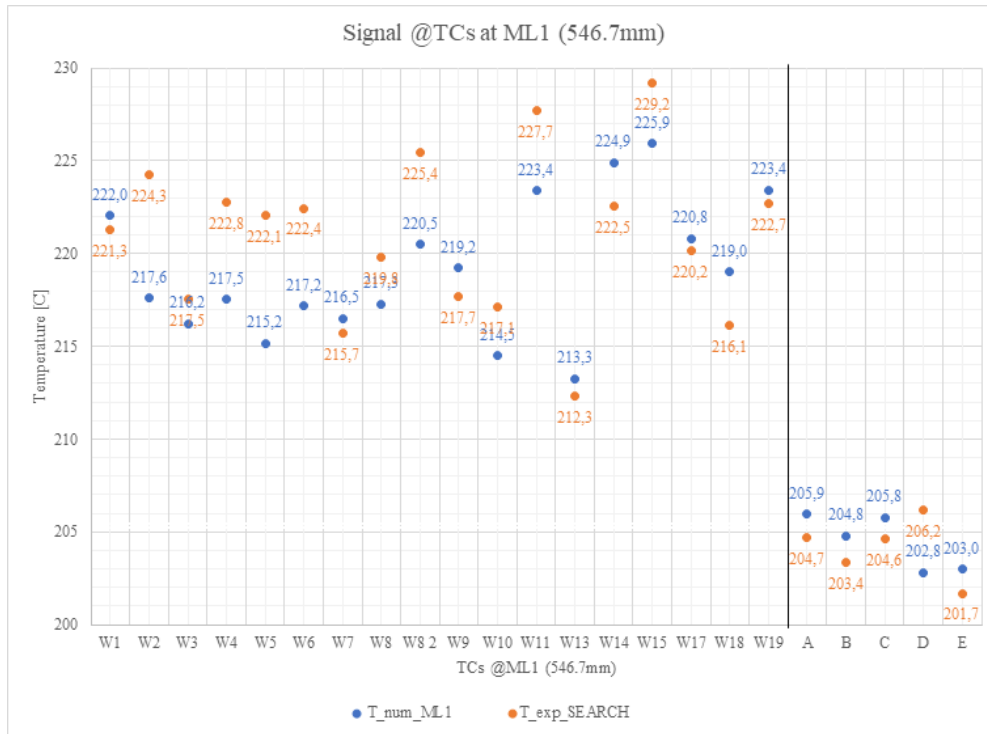


Figure 29 – Comparison of the temperature between the numerical and the experimental values at the TCs placed at ML1 with model setup of Chapter 4

The behaviour of the temperature distribution described previously is even more accentuated in the contour plot of Figure 30 (refer to Figure 26 for the TCs position, labels of which are not represented in the plot below, for sake of clearness), where it is evident that the hottest spots are at the contact point between the wire and the cladding.

These more promising results let to the verification of the good accordance with the general behaviour of the flow inside the fuel bundle, as well as a better prediction of the values of the temperatures at every TCs.

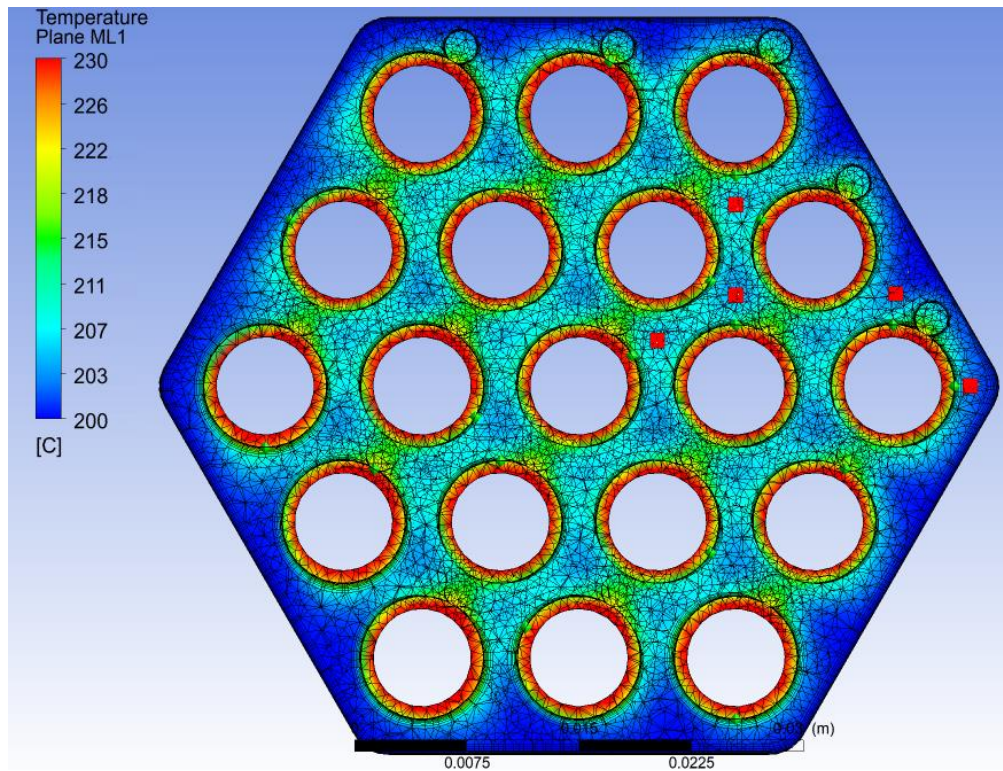


Figure 30 – Temperature contour plot at the ML1 for the unblocked case scenario with model setup of Chapter 4

Proceeding further with the analysis, it is important to highlight that the results present below are considered reliable, because the velocity and temperature values obtained from this simulation has been compared to the results obtained by a model in which the computational domain has been meshed with a very high resolution and refinement (92.1 million cells) which have allowed to reach an average value of y^+ around 2 at the surfaces of the claddings and wires, and 3.5 close to the hexagonal channel boundary. The difference in the values encountered was of 0.1 m/s on the maximum velocity and around 1 K for the temperature.

Here below the results obtained will be presented, each time compared to the experimental data from the tests done in the THEADES loop [45] and the numerical results from NRG [46]. The values were probed at the same TC location as in the experiments, as also NRG has done, and hereunder depicted in three different graphs: at the blockage mid-height, in the wake of the blockage and at the downstream measuring level (see Figure 27).

At the blockage mid-height, as already explained in “Chapter 2 – ” and reminded in the small scheme at the right of Figure 31, five TCs are installed: three are at the interface with the blockage, while the remaining two are facing the liquid LBE. As showed by the results depicted in the figure below, there is an excessive overestimation of the temperatures in correspondence of the

blockage, behaviour observed also by the NRG. The horizontal straight lines are representing the bulk temperature, which in the present model has been evaluated as a mass flow average on the plane, therefore resulting from the energy balance. Although its good agreement with the experimental value of the bulk temperature, evaluated according to Equation 1, suggests that the model is solving correctly the problem, the local values of the temperatures show a big overprediction of the experimental data, even if the value of the temperature is lower compared to the blocked TCs (they are cooled by the liquid LBE).

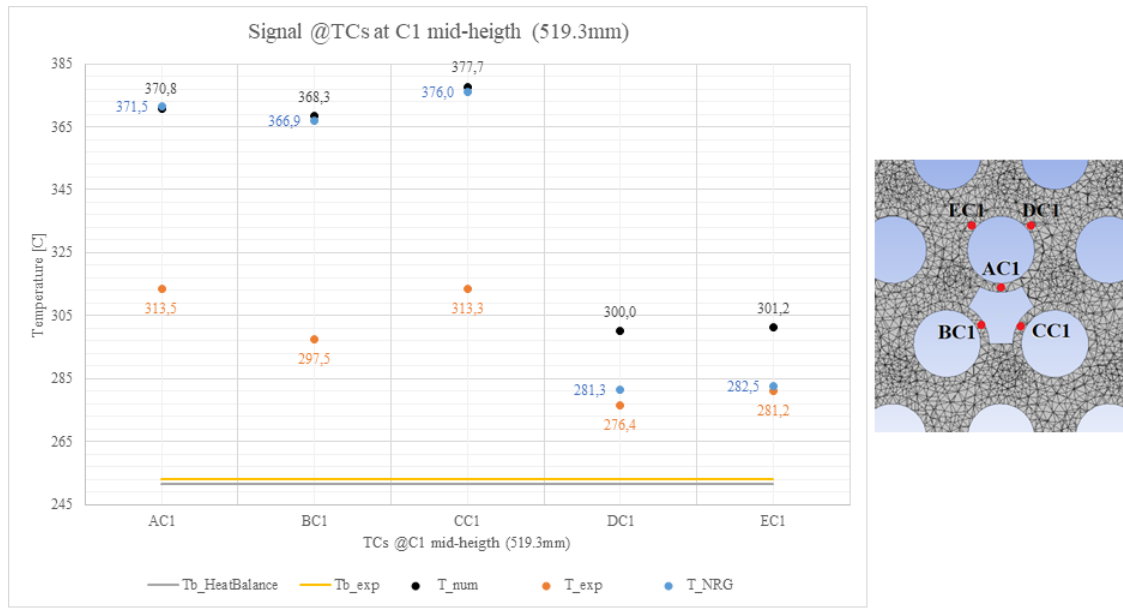


Figure 31 – Comparison of the temperature values evaluated at the TCs at the blockage mid-height between the present analysis, the experimental data and the NRG results

In the wake region, the thermocouples are placed in the bulk of the blocked subchannel, each positioned at of about 18.2 mm downstream the blockage, where the third one corresponds to the one present at the measuring levels indicated above. These locations have been represented by planes at the corresponding axial coordinate in Figure 27. The results represented in Figure 32 show how the temperature recovers in the wake of the blockage, but there is a gap of approximately 25K with the experimental values, as already observed by NRG, even if in all cases the trend is approximately constant. On the other hand, even if the behaviour of the temperature profile is corresponding to the one obtained by NRG, there is a more or less constant offset with their results. This aspect will be discussed later in this section. The bulk temperature, in this case represented by a dashed line, is steadily increasing because the liquid LBE continuously heats up along the fuel bundle.

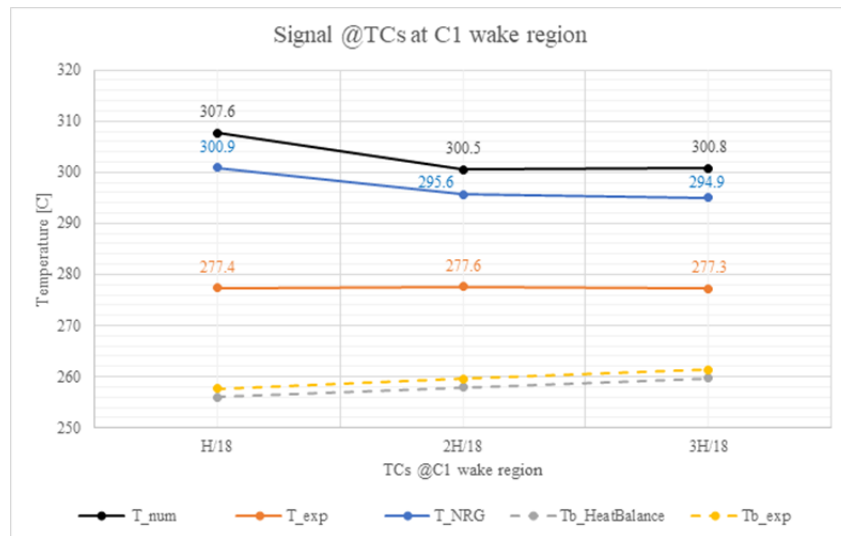


Figure 32 – Comparison of the temperature values evaluated at the TCs in the wake of the blockage between the present analysis, the experimental data and the NRG results

At the measuring level 1/6 wire pitch downstream the blockage the thermocouples can be divided into two groups: the ones embedded into the cladding, on the left of the black line in the graph, and the ones in the centre of the subchannels, on the right. What is visible from the plotted temperatures in Figure 33, there is a general overestimation of the fluid temperatures in the wake of the blockage, and towards the centre of the fuel bundle, while underestimated in the corner and edge subchannels, identified respectively by the thermocouples “E” and “D”. The same observation is drawn for the temperatures taken at the embedded TCs, that are higher for the ones facing the more central subchannels where the fluid temperature is higher.

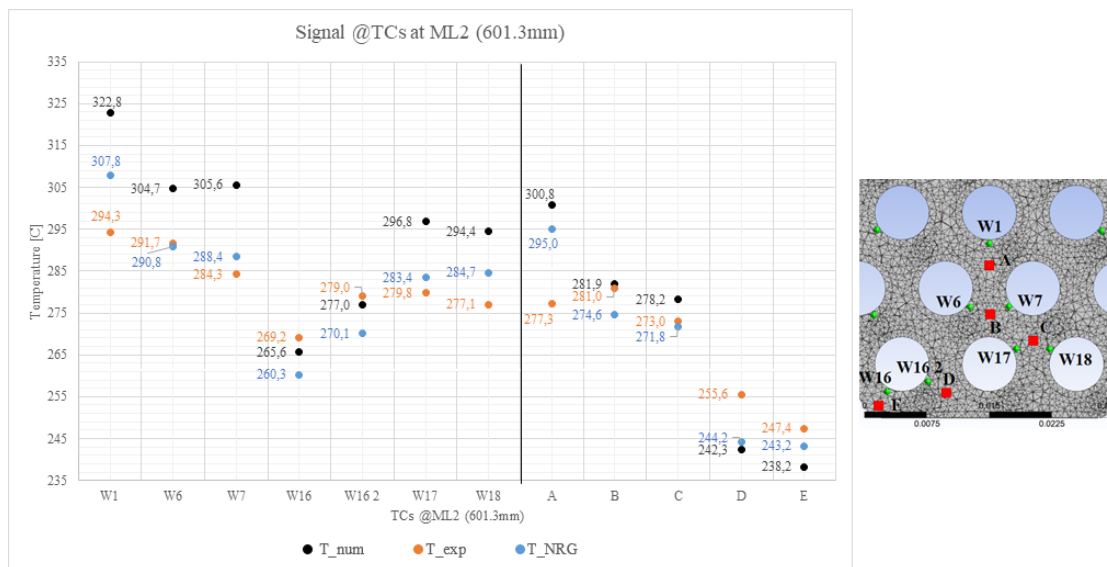


Figure 33 – Comparison of the temperature values evaluated at the TCs at the ML2 between the present analysis, the experimental data and the NRG results

The temperature distribution visible in the contour plot of Figure 34 shows clearly, as it occurs also in the experimental test section and in the prior numerical simulations, that the bulk of the fuel bundle is warmer compared to the external ring, and that as expected the hottest spots are located in the pins which were in contact with the blockage, mostly close to the contact zone with the wire. This same trend has been observed also in the unblocked case scenario, therefore it can be concluded that the effect of the blockage is minor at this distance downstream, i.e. at ML2, because this behaviour is generally observed in the whole channel and not only in the wake of the blockage.

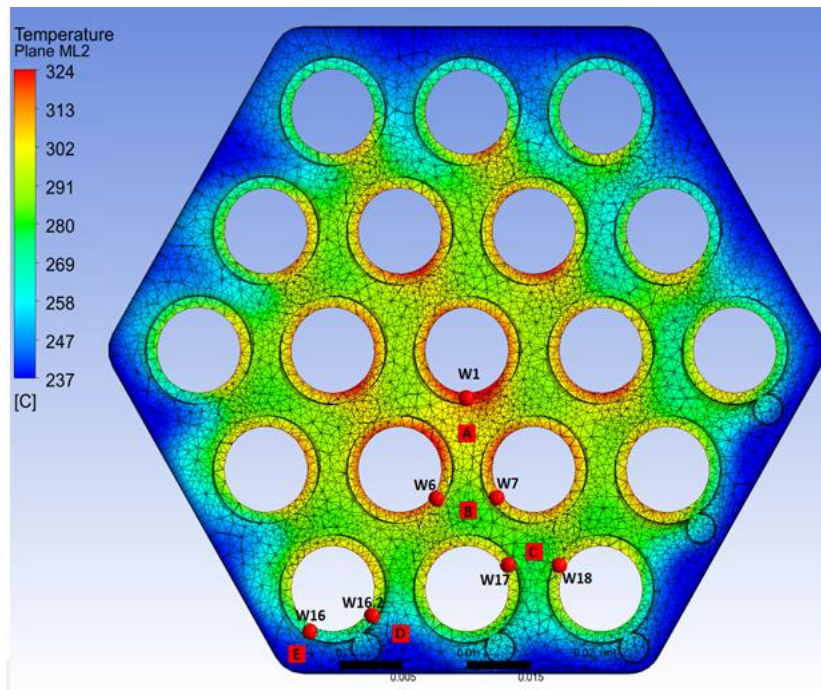


Figure 34 – Temperature contour plot at ML2

Additionally, the temperature profiles are taken along lines passing through the points that correspond to the TCs at the measuring level at the centre of the subchannels are placed (Figure 35), and additionally the one sampled in the blocked subchannel has been compared with the NRG temperature profile taken along the same line. There plots are found respectively in Figure 36 and Figure 37.

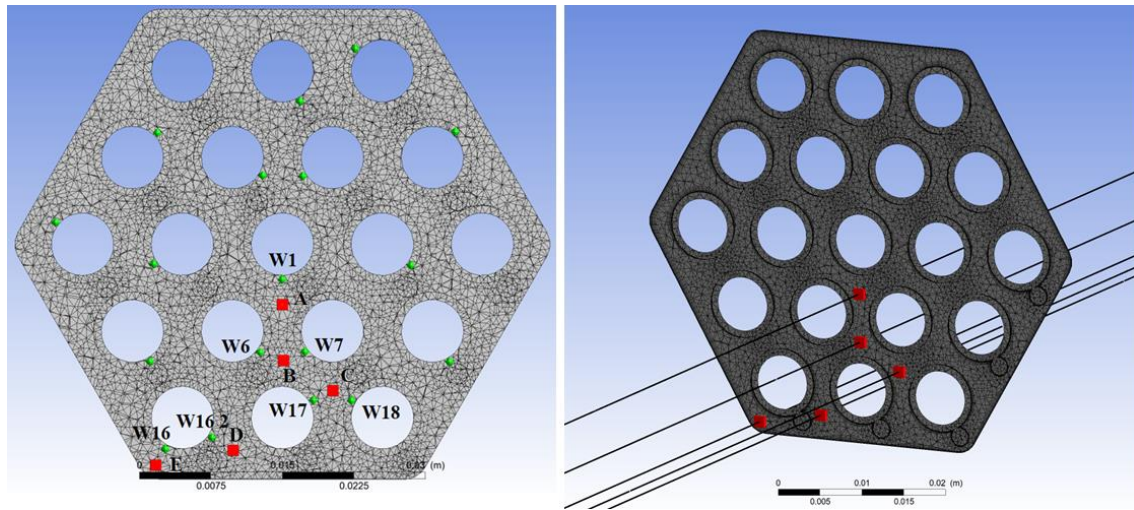


Figure 35 – Specification of the position of the sampling lines corresponding to the TC positioned in the subchannels at ML2

Here below the different profiles are displayed (Figure 36), with the TC positions identified by the dots in the plot: the peaks that are visible on all the profiles are corresponding to the locations where the wire is crossing the lines, therefore the temperatures present a higher value compared to the fluid. In addition, the general behaviour of the profile are confirming what has been stated above, namely the fluid in the subchannels that are in the external ring of the hexagonal channel and therefore close to it (in the plot: green line corresponding to the thermocouple D and blue line corresponding to the thermocouple E) is colder, compared to the subchannels which are instead more in the centre of the fuel bundle (in the plot: pink line corresponding to the thermocouple B and purple line corresponding to the thermocouple C). The steadily increasing behaviour is evidently because of the fact that the fluid is heating up along the channel. For the central subchannel, the temperature decreases downstream the blockage, but it never recovers completely.

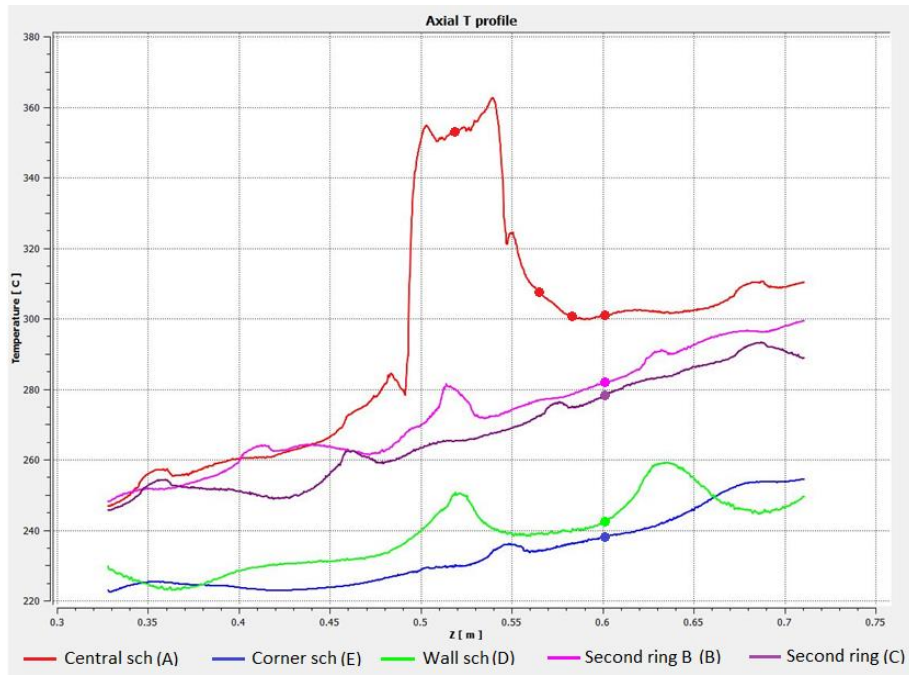


Figure 36 – Temperature profile at the centre of the selected subchannel

Moreover, taking a more detailed look to the behaviour of the temperature in the central subchannel in comparison to the results of the NRG, it is confirmed by the figure below (Figure 37) the good agreement between the CFD models in the prediction of the temperatures in the region of the blockage, where the peaks that are visible are due to the local vicinity of the wire, which hinders even more the eventual cooling by the surrounding fluid. Furthermore, it is clearly visible the constant offset found in the prediction of the temperatures in the fluid domain, which is in the range of 5-10K of difference depending on the location. It is assumed that this difference can be accounted to the different flow development modelling: in this thesis the thermal-hydraulic field is developing in three subsequent computational domains, whereas NRG simulations were run using one single domain. Additionally, this phenomenon might be also explained by the difference turbulence model adopted, as well as the different commercial CFD code used.

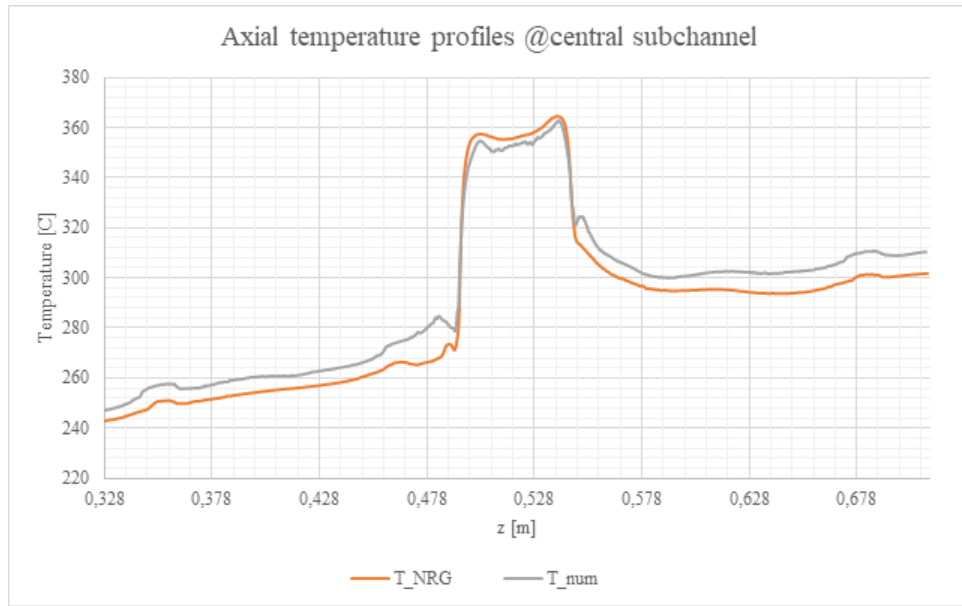


Figure 37 – Temperature profile at the central blocked subchannel

Hence, the analysis that has been done below is pointing towards finding a possible explanation to the difference in the results with both the experimental campaign data and the NRG numerical results that has been seen in the figures depicted above.

4.4 Blocked reference case sensitivity analysis

Given the big discrepancy encountered between the numerical results and the experimental data, meaningful sensitivity studies have been carried out, in order to address the issue and try to find which could be the reason of the mentioned fact.

4.4.1 Influence of buoyancy

First of all, based on the same computational setup described above, the effect of buoyancy has been considered. Indeed, the 19-pin fuel bundle is placed in the vertical direction with upward flow, and therefore it has been considered that the gravitational effect of the change in the density of the liquid LBE due to the temperature could have played a role.

Since this effect is extremely marginal and the trend is the same for all the TCs, for the sake of synthesis only the temperatures at the blockage mid-height are showed as representation of the analysis (Figure 38).

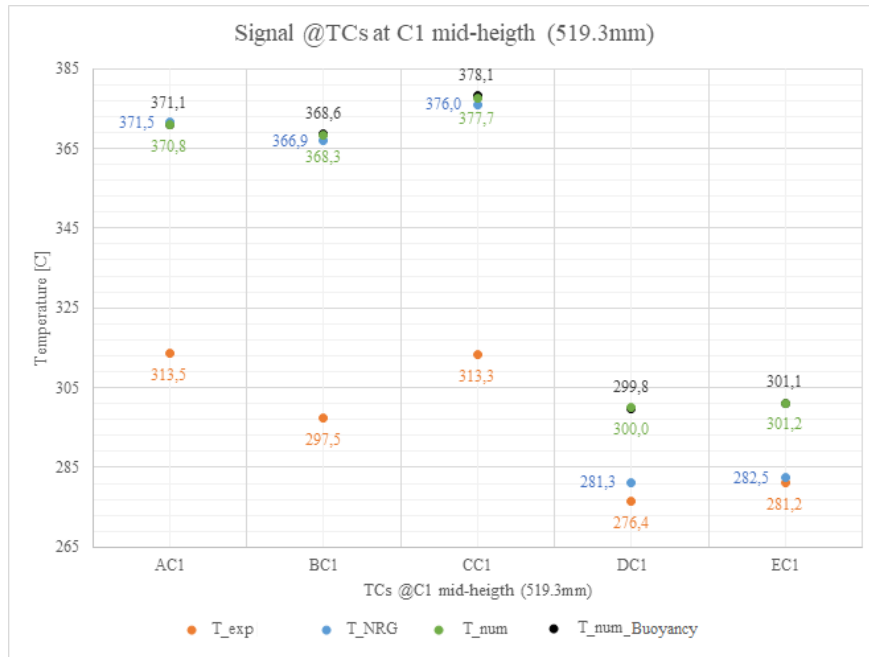


Figure 38 – Effect of buoyancy on the temperature value at the blockage mid-height

As said before, the influence of buoyancy on the temperatures obtained is negligible, because the difference with respect to the simulation without buoyancy the temperature are varying at most of 0.4K, maximum deviation which is encountered at the correspondence to the three TCs adjacent to the blockage. For all the other TCs, the modification is much lower, even for the ones placed in the bulk of the fluid. It can be concluded that the sensitivity to buoyancy is very limited.

4.4.2 Influence of thermocouple position

As it has been done already in the NRG study, also in this analysis it has been considered relevant to investigate which could have been the effect of the variation of the TC position on the temperature values. The reason is the same as already explained above: the majority of the thermocouples are embedded in the cladding wall, nevertheless a certain uncertainty in their exact location could be assumed.

Thus, in order to assess this aspect, the variation in the probing location of the temperature has been implemented with the insertion of small volumes of 0.5 mm in radius around the position of the TCs, so that is has been possible to verify the impact in every direction.

From Table 11 it is possible to see the impact of such variation on the temperatures which are probed in correspondence of the TCs at the blockage mid-height, where the most significant discrepancies with the experimental data and temperature gradients are encountered, and in correspondence of the TCs located in the wake of the blockage in the blocked subchannel, where

the highest uncertainty in the TC position is expected, since they are installed in the bulk of the fluid. The position of the TC is once more reminded in the representation below to the table, where the dimension of the points have been exaggerated for sake of clarity (Figure 39). It is important to mention that it has been verified that the temperature probed were considered in the domain in which the thermocouples are probed, accordingly as it has been done in the previous works.

TC	Domain	ΔT [K]
AC1	cladding	3.9
BC1	cladding	3.5
CC1	cladding	3.2
DC1	cladding	4.0
EC1	cladding	3.3
H/18	LBE	2.1
2H/18	LBE	4.8
3H/18	LBE	3.0

Table 11 – Effect of the probing position on the temperature value

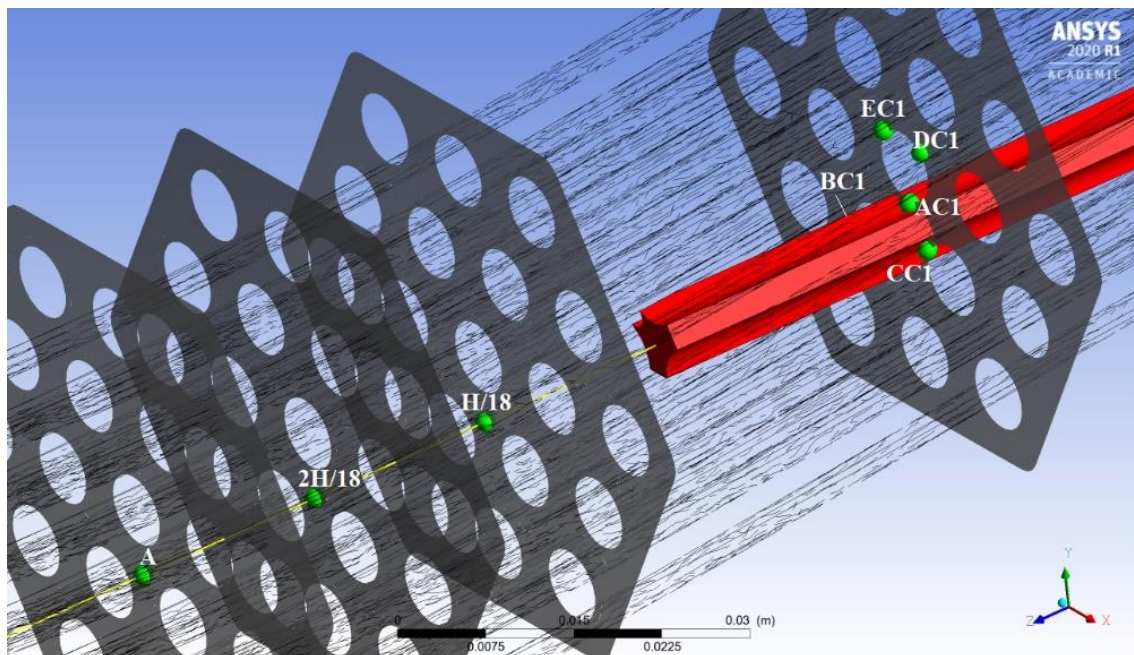


Figure 39 – Blocked domain close-up with specific representation of the location of the TCs

Although the still relatively big mesh element size and the radius of the volume that is of comparable size of the cladding thickness, the temperature difference obtained for the different TCs is small (less than 5K).

Therefore, it can be concluded that since such a big variation in the TC position cannot be present in the experimental setup, the difference in the temperature values considering a much smaller variation has to be negligible, and consequently the much larger discrepancy with the experimental data cannot be accounted to this situation.

4.4.3 Influence of the turbulence model

Despite the initial choice of the turbulence model, which has been done because its better performance in these types of flow conditions has been proved based also the previous experience found in the literature [51][66][67], it has been chosen to modify it, as well as the Turbulent Pr number, in order to simulate the same conditions that have been imposed by the NRG to have a more consistent comparison with the results they obtained.

Thus, in specific, the turbulence model has been changed from $k-\omega$ SST to standard $k-\epsilon$, and the Turbulent Pr number has been set equal to 2.

As it is visible in the figures below, there are two unexpected outcomes for this analysis. First of all, even if with the value of the y^+ obtained in this simulation the resolution of the $k-\epsilon$ model with automatic wall function should be more consistent, as explained in “Appendix B – Numerical modelling theory”, the sensitivity of the model to this change is very limited. Indeed, compared to the model with $k-\omega$ SST, the difference in the temperatures encountered is at most of 4°C (Figure 40), value measured at one of the blocked TC at the blockage mid-height, whereas it is less than 2°C at the TCs in the bulk of the fluid, where the effect was expected to be more significant (Figure 41).

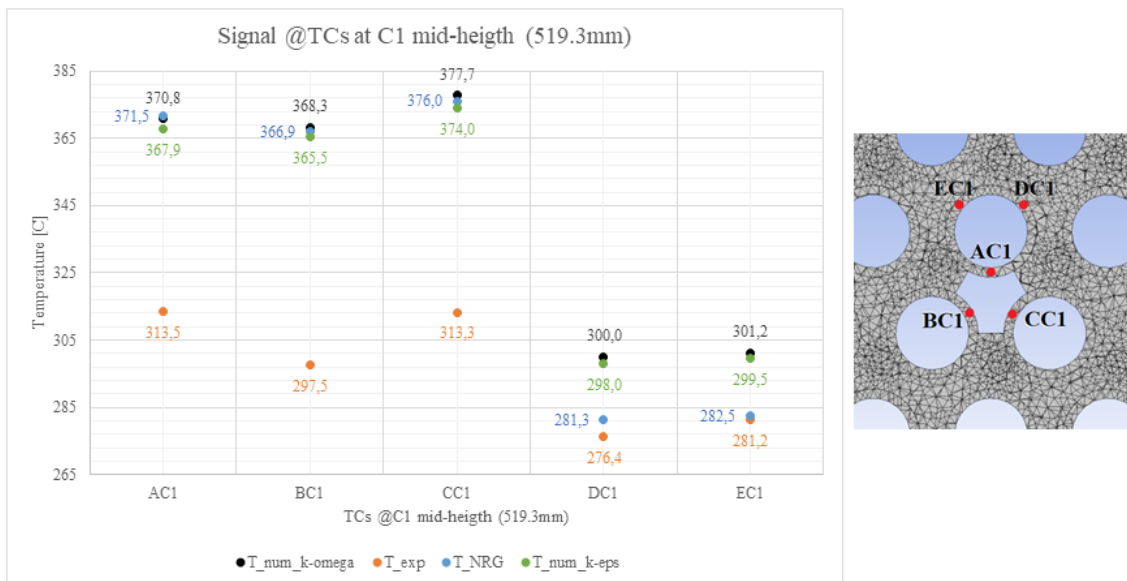


Figure 40 – Effect of the turbulence model on the temperature value at the blockage mid-height

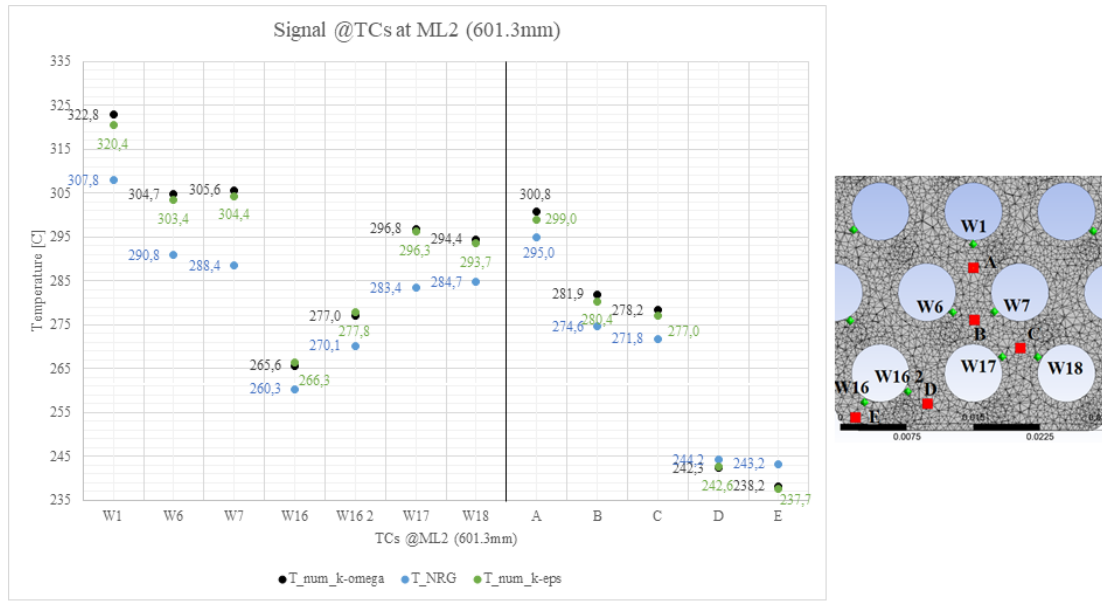


Figure 41 – Effect of the turbulence model on the temperature value at ML2

This phenomenon is confirmed also by the comparison between the velocity profiles obtained by the implementation of the two different models, taken along the line in the bulk of the central blocked subchannel (yellow line in Figure 39), as depicted in Figure 42. Indeed, although the slight difference in the zones right before and after the blockage, the behaviour is very similar all along the domain, even for the recirculation zone downstream the blockage (where the values of the velocities is negative). It is important to mention that the velocity is evidently zero where the line is crossed by the wires and the blockage. Thus, given these results, it can be concluded that the model under analysis shows little sensitivity to the change in turbulence model.

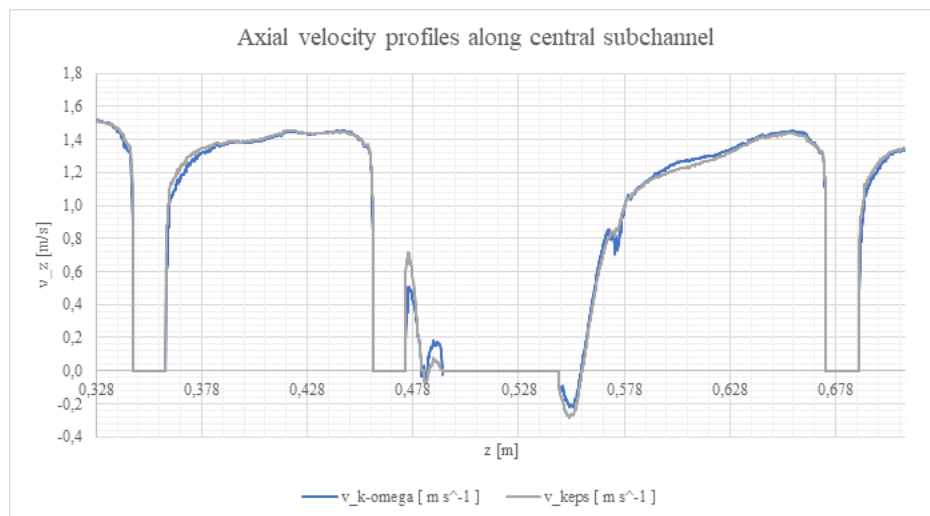


Figure 42 – Comparison of the velocity profiles between the two turbulence models implemented

The second unexpected outcome, as visible also in Figure 43, the implementation of the $k-\epsilon$ turbulence model and the modification of the Turbulence Pr number did not show the effect that it has been supposed. Indeed, the results obtained with this parametric study present still an offset with respect to the NRG values, albeit the same conditions and setup have been imposed. It is true that the difference with the temperature values obtained by NRG is relatively small in the bulk of the fluid (below 5°C), but for the TCs embedded in the cladding reaches even 15°C in some locations. This cannot be accounted to the materials used, since they are the same, therefore it is assumed, as mentioned before, that the cause might be the different implementation of the same turbulence model by the different commercial codes. Besides, it has to be mentioned that a different mesh methodology has been implemented and the development of the fluid profiles is different for the two analysis, as explained before. All these aspects might have an impact on the offset between the two simulations here compared.

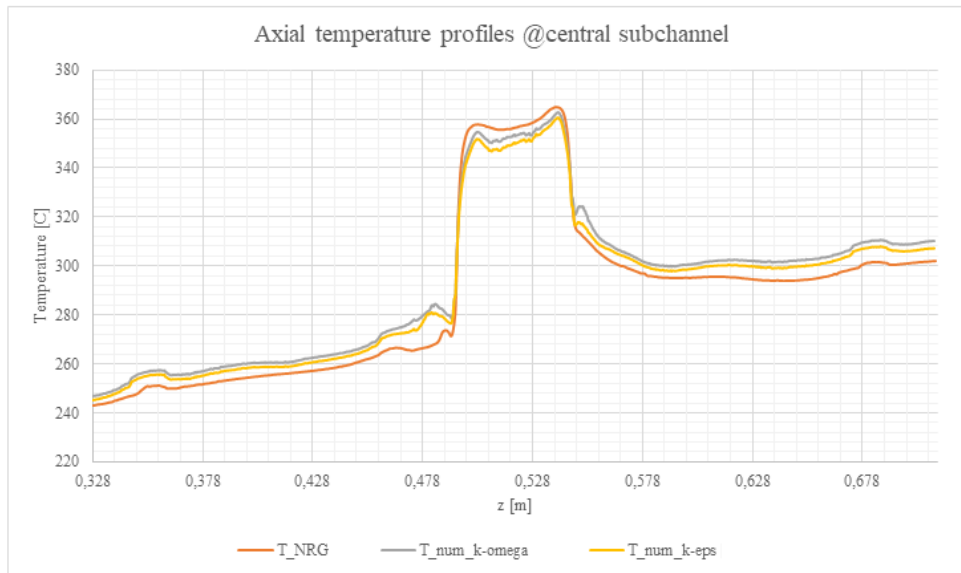


Figure 43 – Comparison of the temperature profiles between the two models implemented

4.5 Blockage refinement model

In the present section the model, in which the region of around the central blockage has been investigated in detail, will be presented. The reason of the reduction of the domain to a region surrounding the blockage has been driven by the necessity of a deeper investigation on the issues presented above, and therefore a smaller domain allowed for a bigger refinement of the mesh in the region under investigation, still maintaining a reasonable computational cost.

Here below the modified domain will be explained, with all the setup changes implemented in the computational domain that has been taken into account in this chapter in order to achieve the

desired model, as well as the sensitivity analysis done, again with the purpose to investigate the difference with experimental data and try to identify the reason of the big discrepancies in the prediction of the temperatures at the blockage.

4.5.1 Computational domain settings

As mentioned before, given the fact that this model is the refinement of the region surrounding the central blockage, the geometry on which it is based and the materials used are the same as the ones that have been already discussed previously in this chapter (section “4.1 Base case geometry modification and materials”), namely the 19-pin wire-wrapped fuel bundle encased in an hexagonal channel.

The computational domain instead has been reduced significantly, since the zone under analysis is a smaller portion of the original one. As visible in Figure 44, the original domain has been cut in a hexagonal shape centred around the blockage, involving then the three adjacent pins and a 60° sector of three other pins. The domain is 1/3 wire pitch long and contains completely the blockage, allowing some space both upstream and downstream the blockage.

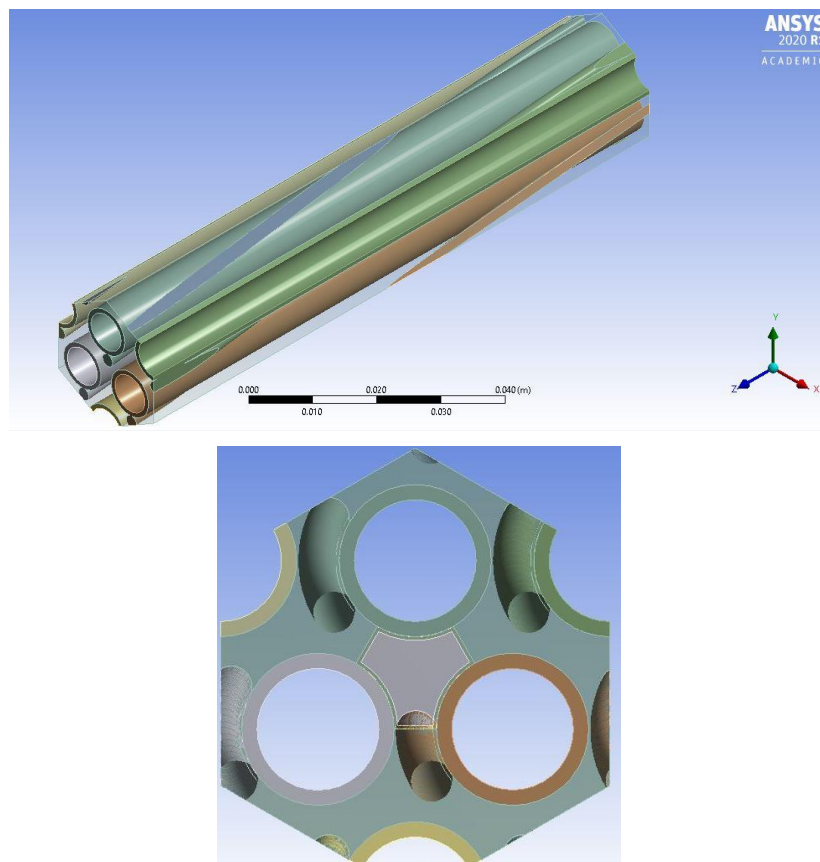


Figure 44 – Computational domain of the refined blockage region model: complete geometry (above) and cross-section at the blockage mid-height (below)

As far as the meshing is concerned, the fluid volume is once again meshed with an unstructured mesh of tetrahedrons, whose size has been decreased compared to before, in order to have a more refined mesh in the bulk. The inflation layer, this time only at the walls of the claddings and wires, is still composed of several layers of prisms in order to capture the near-wall phenomena. What has been changed compared to before is the mesh inside the central pins and in the blockage as well, which in this model is structured (Figure 45).

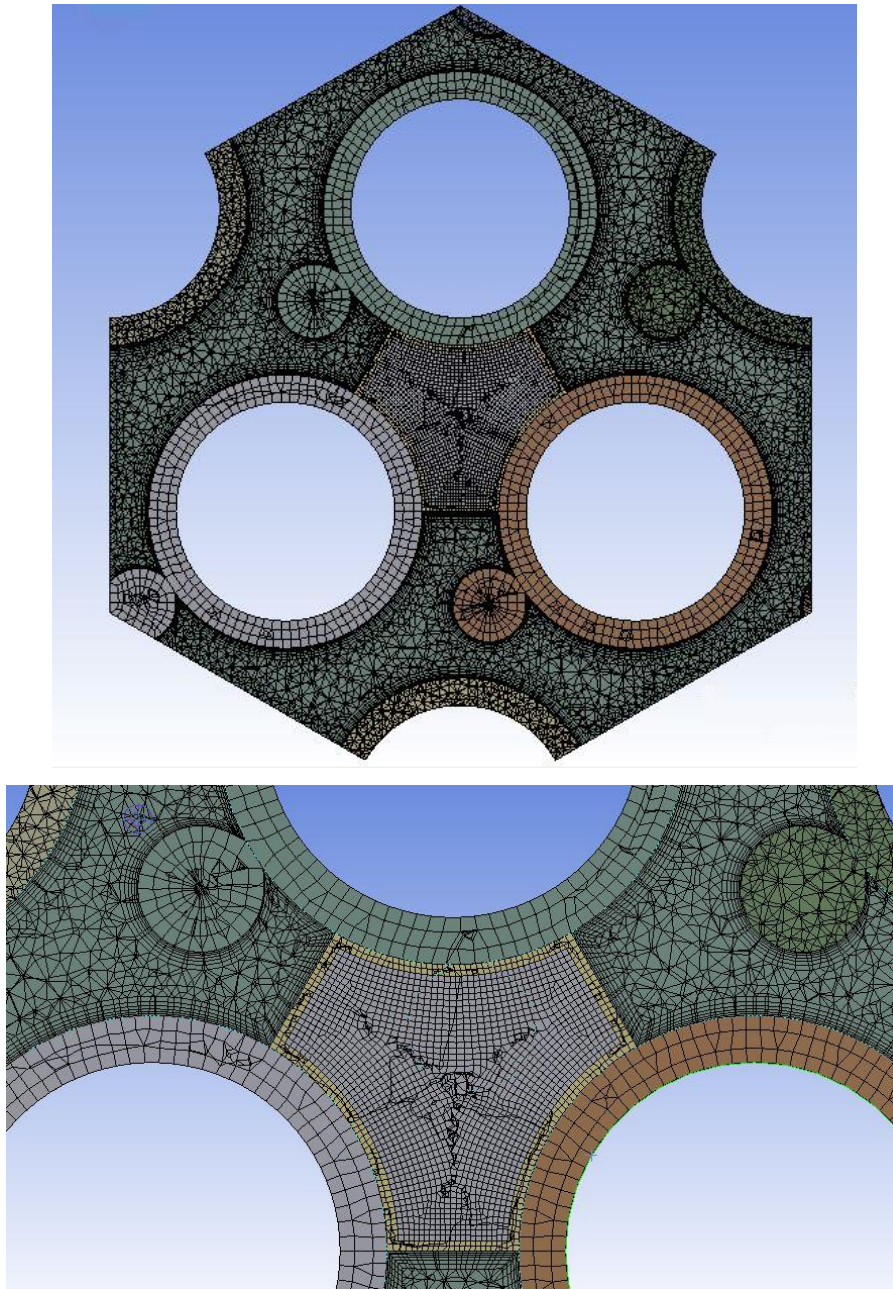


Figure 45 – Mesh of the cross-section of the 19-pin wire-wrapped fuel bundle of the refined blockage domain: whole cross-section at the outlet (above) and close-up at the blockage mid-height (below)

The computational setup has been summarised in the table below (Table 12):

Methods	Standard k-ε (RANS), Turbulent Pr = 2	
Time dependence	Steady state	
Domain	Surface	Boundary condition
Fluid (LBE)	Faces on hexagonal boundary	Translational periodicity boundary condition
	Inlet	$\dot{m}_{in} = 15.54 \text{ kg/s}$ $T_{in} = 200^\circ\text{C}$
	Outlet	p_{out}
Solid (SS 1.4571)	Internal rod surface	$q'' = 0.580 \text{ MW/m}^2$
	Wires and external cladding surface	Conservative interface flux with LBE and blockage
Central blockage	Paste and shell	Conservative interface flux with LBE, claddings and wires
Total N# cells	9.1e6	
N# cells in fluid (LBE)	5.9e6	
N# cells in cladding and wire	1.9e6	
N# cells in blockage	900.5e3 (paste) 421.2e3 (shell)	
Avg y+ cladding and wire	10.6	

Table 12 – Refined blockage domain model setup specification

It is relevant to point out firstly that the choice of turbulence model has been done given the conclusions obtained before, namely the low sensitivity that the previous model has showed to such a modification. Additionally, by doing so, all the results obtained could be directly compared to the ones by NRG.

In the second place, it is highlighted the fact that the boundary conditions imposed were all of “profile” type: at the inlet boundary the velocity profile, the relative turbulence parameters and the temperature profile have been imposed, all of them retrieved at the correspondingly axial location from the complete domain described in section “4.2 Blocked reference case”. Similar procedure has been applied for the outlet boundary, where the pressure profile has been imposed. Moreover, as it has been specified in the table above, the sides of the domain, which are structured in a hexagonal geometry, have been coupled in three pairs of oppositely facing sides and on each of them a periodic boundary condition has been set, in order to simulate the circulation of the

flow. In the same fashion as for the other models, the heat flux (q'') is uniformly distributed on the internal surfaces of the rod cladding.

It is important to mention at this stage that the results obtained with this refined model have been compared with the ones of the entire domain, in order to verify that the assumptions done were pointing in the right direction, and are briefly discussed here below.

Figure 46 confirms that the setup of the model is physically representing the phenomena, since there is a good agreement with the temperatures at the TCs that have been obtained from the previous model. Moreover, the velocity profiles in Figure 47 (retrieved on the same line at the centre of the blocked subchannel represented in Figure 39) are also similar to the complete domain, therefore it can be concluded that the results obtained in the previous discussion are mesh independent.

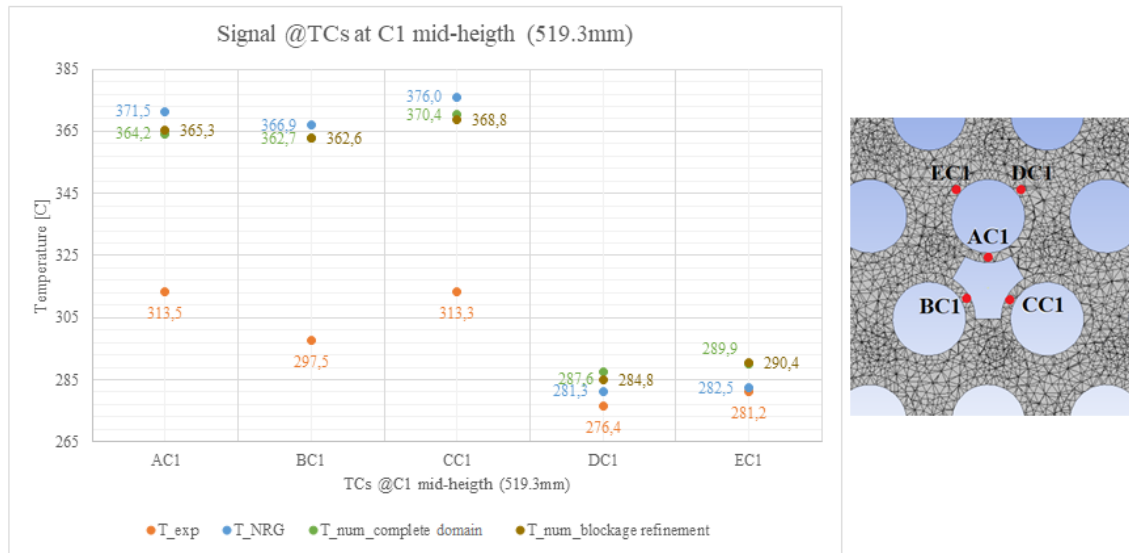


Figure 46 – Comparison of the temperature values at the blockage mid-height between the refined blockage domain and the complete domain



Figure 47 – Comparison of the velocity profiles along the line at the centre of the blocked subchannel between the refined blockage domain and the complete domain

Given these conclusions, in the next paragraphs some modifications have been implemented, in order to tackle the above-mentioned issue.

4.5.2 Influence of the turbulence model

Since a previous variation of the turbulence model has been already tried for the entire domain, showing a small sensitivity to it, in this case another turbulence model has been applied: the BSL Reynolds Stress Model, model that has been described in “Appendix B – Numerical modelling theory”.

Although the promising characteristics of this model, it is visible from Figure 48 that in the case under analysis it doesn’t bring a significant improvement, probably accounted to the implemented unstructured mesh, which could not be suited for such turbulence model. Indeed, the sensitivity to such model is negligible or even going in the wrong direction, showing a higher discrepancy with the experimental data, and therefore it doesn’t justify the higher computational cost required for the resolution of the additional equations that this type of model foresees.

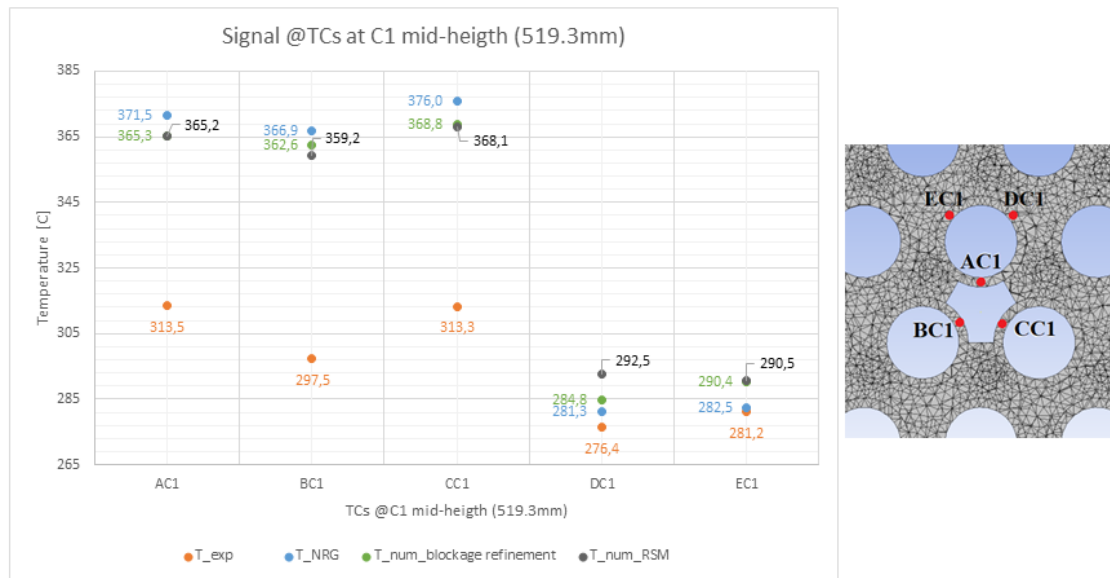


Figure 48 – Effect of the turbulence model on the temperature value at the blockage mid-height in the refined blockage domain

4.5.2 Influence of the inflation layer refinement

The additional verification that has been done was the effect that a more refined mesh at the vicinity of the pins cladding and wire surfaces would have given to the results.

In specific, the refined mesh of the reduced domain surrounding the blockage that has been described above was modified in the following way: the core mesh settings are kept the same, while only the inflation layer has been modified, decreasing the thickness of the first cell and setting a number of layers and growth rate (the value that identifies the rate at which the cell thickness increases at each subsequent layer in the radial direction) which allowed for keeping the original inflation layer total thickness.

The cross section of the mesh can be seen in Figure 49 and the specifics in Table 13.

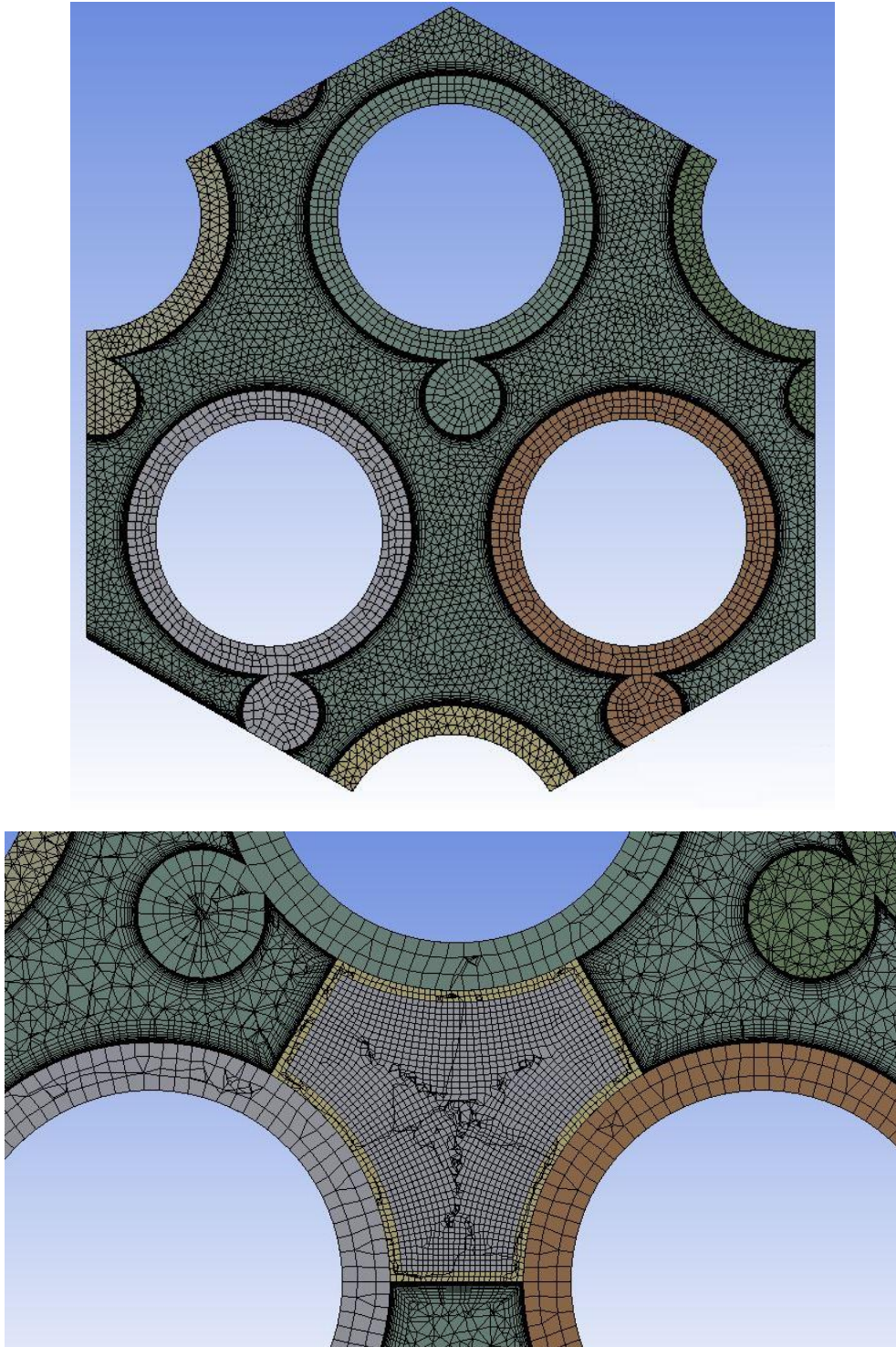


Figure 49 – Mesh of the 19-pin wire-wrapped fuel bundle of the refined blockage region model with refinement of the inflation layer: whole cross-section at the outlet (above) and close-up at the blockage mid-height (below)

1st layer cell height	5e-6 m
Maximum N# layers	13
Growth rate	1.27
Total N# cells	12.1e6
N# cells in fluid (LBE)	8.9e6
N# cells in cladding and wire	1.9e6
N# cells in blockage	900.5e3 (paste) 421.2e3 (shell)
Avg y+ cladding and wire	2.1

Table 13 – Specifics of the generated mesh

Unfortunately, from the comparison with the results previously obtained for the refined blockage domain visible in Figure 50, it is possible to conclude that even with this very detailed mesh at the wall there is very little sensitivity in the domain, even where it was expected to see a bigger impact, namely for the temperatures at the TCs placed on the central rod, but in the unblocked position (in the figure below “DC1” and “EC1”). Indeed, the difference found in the temperature values is of at most 1K. Besides, since standard k- ϵ uses an adaptive wall function to resolve the boundary layer region and the refinement of the inflation layer might not have an impact, k- ω SST has been imposed to verify the observation just done. Surprisingly, even with the implementation of a model known to perform accurately in this type of flow [68], the drawn conclusion is confirmed: the prediction of the temperature value is not sensitive to the refinement of the inflation layer. Indeed, in this specific case the maximum temperature difference encountered with respect to the results of section “4.2.4 Results” is below 2K.

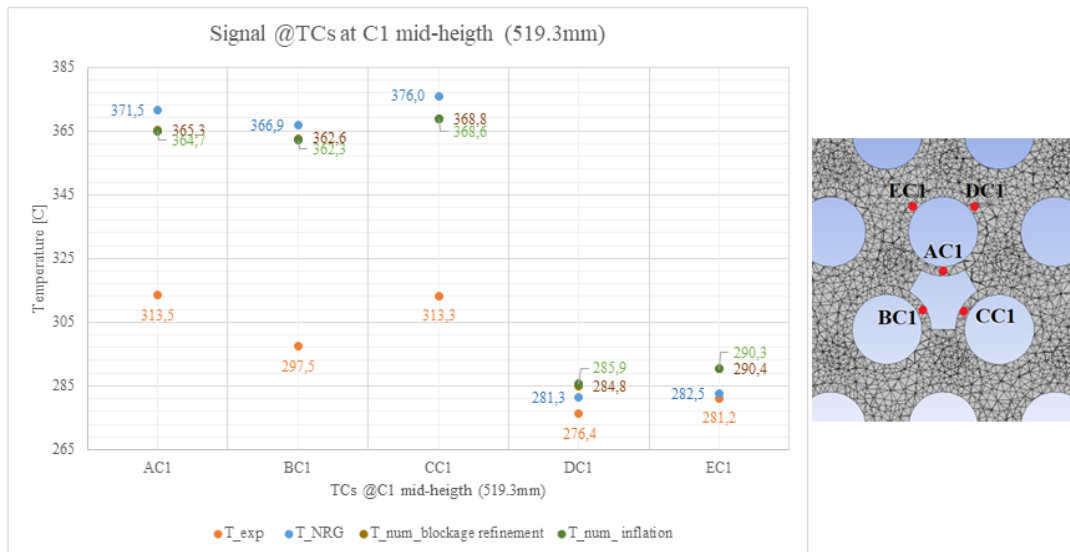


Figure 50 – Effect of the inflation layer on the temperature value at the blockage mid-height in the refined blockage domain

Besides, from Figure 51 and Figure 52, representing the comparison respectively in the velocity and temperature profiles taken along the line at the centre of the blocked subchannel, the same observation done can be drawn.



Figure 51 – Effect of the inflation layer on the velocity profile along the line at the centre of the blocked subchannel in the refined blockage domain

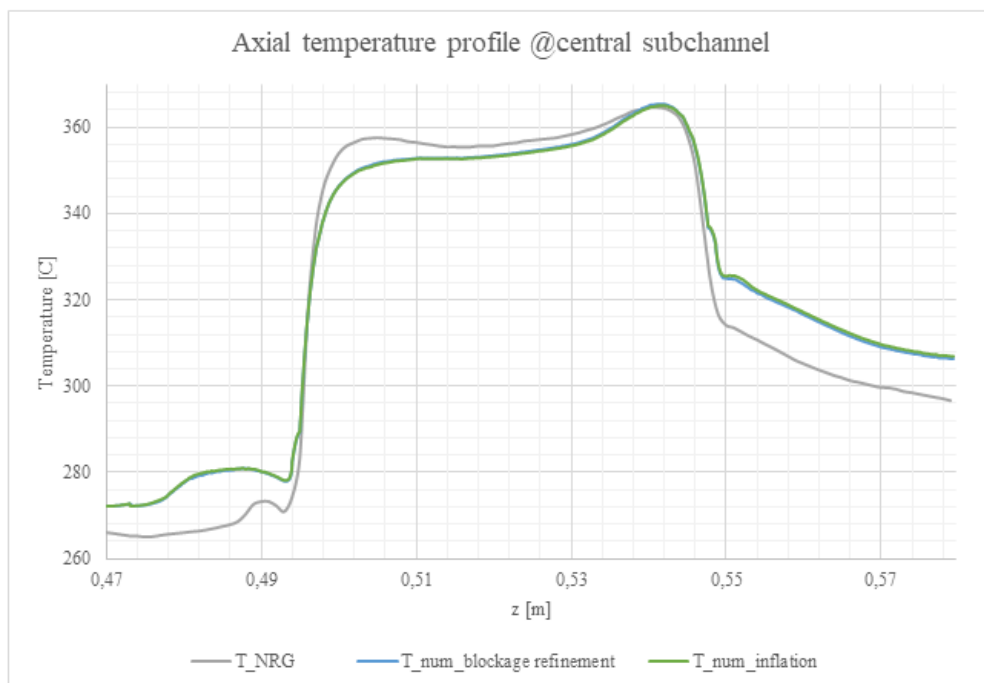


Figure 52 – Effect of the inflation layer on the temperature profile along the line at the centre of the blocked subchannel in the refined blockage domain

It can be concluded that the limited improvement thanks to mesh refinement cannot address the discrepancy in the values with the experimental data, and consequently the increased computational cost cannot be justified. Therefore, it has been assumed that the reason that can eventually describe such difference has to be investigated through different assumptions, as explained in the next section.

4.5.5 Influence of the internal electrical heater modelling

In the experimental setup, in order to apply the heating to the 19-pin wire wrapped fuel bundle, an electrical heater has been inserted inside the rods for the whole heated length extension. In specific, as visible in Figure 53, the cylindrical inconel heater is placed between two layers of boron nitride electrical insulators, with a central copper wire that provides the electrical connection to the heater.

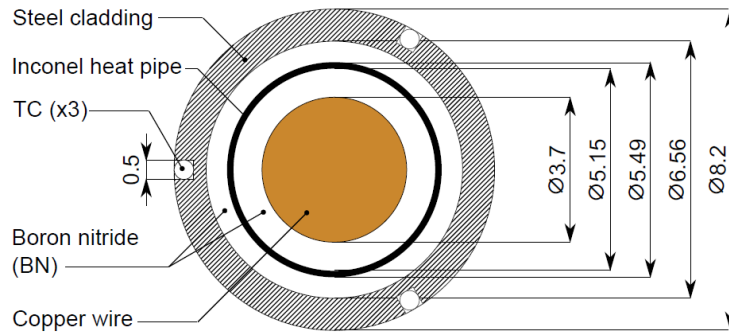


Figure 53 – Cross section of the heated rod (the dimensions are expressed in mm) [45]

A separate simulation has been carried out with ANSYS Mechanical in order to model the electrical heater previously described to verify which were the physical phenomena occurring as a consequence of the presence of the blockage.

The heater element has been simulated with a temperature dependent resistivity. The output of the model has confirmed that the temperature increase due to the presence of the blockage creates an additional electrical resistance, which in turn causes a non-uniform azimuthal distribution of the current density inside the electrical heater at the height of the blockage. This change is only of about 1%, so it leads to a small local power change. Nevertheless, the heat flux on the inside of the cladding in the direction of the blockage is affected much more due to the higher thermal resistance to the blockage compared to the fluid side. This means that the conduction within the heating element through the copper and the electrical shielding modifies heat flow.

Consequent to these observations, the electrical heater has been included in the CFD model, in order to verify the impact of the non-uniformity of the heat flux distribution at the inside of the

cladding on the temperature values. As the temperature effect on the current density is small, a uniform volumetric heat source has been applied to the electrical heater domain, since it is not possible to set the current and voltage conditions in the CFD simulation.

Here below the contour plot of Figure 54 shows the non-uniform distribution of the heat flux on the internal surface of the claddings: it is evidently depicted that the value of the heat flux decreases of about 1.5 times at contact region with the blockage.

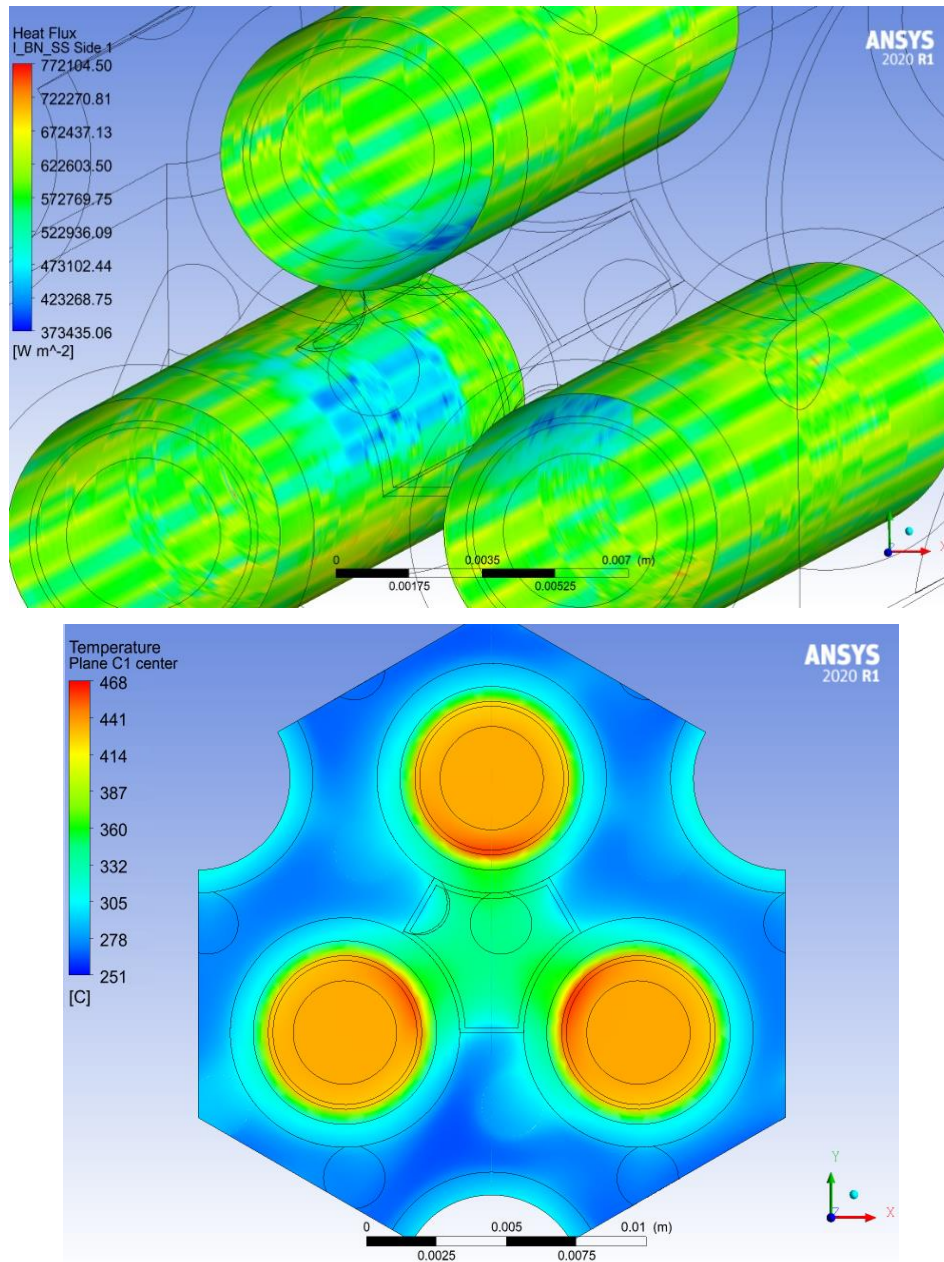


Figure 54 – Heat flux distribution on the internal surface of the claddings (above) and temperature contour plot at the blockage mid-height (below)

In Figure 55 the temperatures taken at the mid-height of the blockage are plotted: it is clear that the non-uniform distribution of the power inside the electrical heater has an effect on how the heat is transferred inside the pin, and therefore the temperature values are affected as well. Although the difference with the experimental data is still big (around 40-50K), the sensitivity to this modification is noticeable and a decrease in the temperatures in the solids is about 11K with respect to the simulation where the uniform heat flux was imposed at the internal surface of the claddings (brown points in the plot), while as expected there is negligible influence on the fluid temperature, visible from the temperature at the TCs facing the fluid.

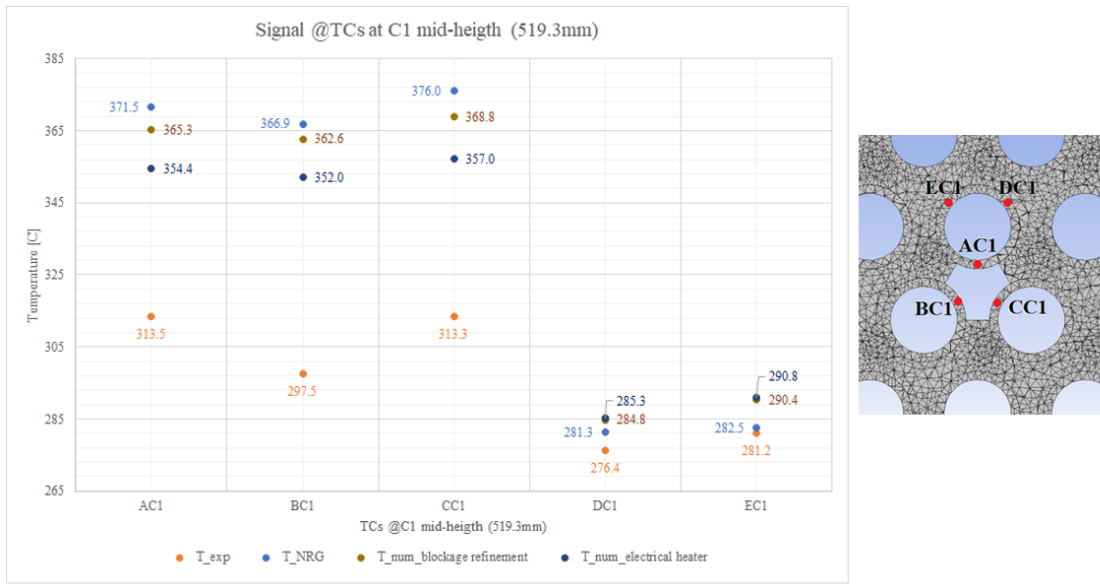


Figure 55 – Effect of the non-uniformity of the heating on the temperatures at the TCs positioned at the blockage mid-height

To conclude, it is relevant to mention that given the results obtained, it is assumed that a bigger impact can be reached in case there would be the possibility to combine the electrical heater model and the CFD one, since it will then be possible to bring together the correct boundary conditions for the fluid domain and the correct modelling of the electrical instrumentation.

4.6 Conclusions

In the chapter here above discussed, the blocked case scenario of the 19-pin wire-wrapped fuel bundle have been discussed instead. As it has been done already before, the procedure used has been explained, presenting the details of the assumptions made, the geometry and mesh used, as well as the computational setup has been described.

The results obtained from this model of the blocked case scenario of the 19-pin wire-wrapped fuel bundle are compared to the corresponding experimental data deriving from the experimental campaign within the European project MAXSIMA at KIT-KALLA where the tests have been performed on an unblocked test section [45] and the numerical results from NRG [46]. These, as it already happened to the previously done simulations, describe properly the general behaviour of the liquid LBE inside the hexagonal channel, nevertheless they show the already encountered issue: the numerical model is significantly overestimating the temperatures at the blockage, while depending on the radial location in the fuel bundle, they either overestimate (towards the centre) or underestimate (towards the boundary) the temperatures at the TCs position.

For this reason, a series of sensitivity studies have been done to address the issue encountered and try to assess the reason that can eventually explain such a discrepancy. The analysis performed covered the influence of buoyancy, the effect on the temperature value with the probing position and the turbulence model used. Unfortunately, the model showed very little sensitivity to all of these evaluations, therefore it was not possible to ascribe the gap in the values to these parameters. In fact, the difference with the experimental data is around 70 K, therefore changes in the temperature difference which are below 5 K are considered negligible when we are in the framework of analysing the sensitivity of certain parameters, also considering the fact that the uncertainty affecting the experimental data is relatively low (± 0.1 K).

Consequently, it has been considered useful to build a model in which only a limited region surrounding the blockage has been considered and therefore investigated in detail. As it has done previously, also in this case the procedure used has been explained, presenting the details of the assumptions made, the geometry and mesh used, as well as the computational setup has been described.

After checking that the model was properly describing the occurring phenomena and that the assumptions done were justified, another set of sensitivity analysis have been performed. In the first place, another turbulence model has been tried and a mesh refinement at the near-wall region has been implemented as well. Unfortunately, in both cases the effect on the results has been marginal, suggesting that the that the difference between experimental and numerical results can't be ascribed to the characteristics of the model, but that the reason might be found in the physics of the problem.

This assumption lead to the investigation of the effect that the modelling of the internal parts of the heater elements could have on the results. Indeed, the 19-pin wire-wrapped fuel bundle is

electrically heated in the experimental campaign, therefore in the simulation described the electrical instrumentation has been added. The model showed a higher sensitivity to this implementation, also confirming that the heat flux at the internal surface of the cladding is not uniformly distributed as it has been assumed from the beginning. Indeed, on the contrary, the additional thermal resistance introduced by the presence of the blockage leads to a variation in the distribution of the heat flux. This is because the effect of thermal conduction into the electrical insulation material and into the copper wire causes a preferential heat flow towards the least resistant path to fluid and not to the blockage.

To conclude, the complexity of the problem is clear: in the first place the geometry of the 19-pin wire-wrapped rod bundle is difficult to be represented precisely in a CFD model, due to the occurring issues related to the meshing of the contact points between the rod and the wire. Besides, also the very tiny dimensions create modelling complexities in the contact regions of the blockage and the adjacent rods, not to mention that CFD models for the simulation of the heat transfer in liquid metals are still under development.

Although all these complexities are surely causing uncertainties in the numerical work done, it is recommended to investigate further the effect of the non-uniform heat flux by the combination of the observations obtained by an electrical model and the numerical characteristics of the modelling of liquid LBE in a CFD model.

Besides, also experimental complexities are not negligible: the complexities of the construction of the test facility, like the fixation of the rods and their relative position with respect to the hexagonal channel, the exact location of the thermocouples and the insertion of the of the blockages within the bundle, must be taken into account. In these regards, it is believed that a further investigation should be made on a remark mentioned in the results from the SEARCH experimental campaign [58]. In specific, it is mentioned in the work that the energy balance made was indicating that the estimated thermal power was 3–5% larger than the measured electrical power. Although this discrepancy was accounted to the uncertainty on the recommended correlation for the specific heat capacity (c_p), it might be also accounted to eventual heat losses of the test section, given the difficulty of obtaining perfect adiabaticity at the walls of the hexagonal channel. If this would be the case, the imposition of an adiabatic boundary condition in the numerical model would not appropriately represent the physical phenomenon, since no heat transfer with the walls is allowed.

Chapter 5 – Fuel assembly model with porous blockage

Until now the analysis took into account the worst-case scenario, where the postulated blockage scenarios conservatively involved complete solid blockages. In this chapter the assumption will be relaxed, since a certain porosity could be expected in case the initiation mechanism of blockage elements is considered to be by accumulation of particles around the wires in the longitudinal direction, like PbO or fuel pellet fragments after cladding failure. In this latter mentioned case, such particles would also emit heat.

In the present chapter the effect of porosity and self-heating of the blockage on the fluid flow will be analysed, since local partial blockages of this type are considered more probable to occur during the operation of LMFBR. Therefore, it is of paramount importance to investigate the risk of their presence in the lead-cooled fuel bundle in order to assess the safety of the installation.

5.1 Fuel bundle with porous blockage model

Taking into account the modelling process thoroughly explained in the previous chapters and the related results discussed, it has been considered more appropriate to implement the modifications and to set the parametric study on the refined blockage domain model explained in section “4.5 Blockage refinement model”. Therefore, the geometry and the materials used are unchanged with respect to what has been already explained in “Chapter 4 – Fuel assembly model with solid blockage”.

As it has been done previously, a step by step approach has been implemented: at first only the steel blockage shell has been changed into a porous material, secondly a complete porous blockage has been modelled, and finally self-heating has been added to the element.

As far as the computational setup is concerned, it is important to describe the rationale behind which all the assumptions are made. The principal starting idea has been to imitate the process applied by NRG work [46], in which a leakage path between the rod cladding and the blockage casing has been modelled by replacing the steel material of the blockage casings with liquid LBE. For this reason and in order to compare the numerical results obtained by the two approaches, the same setup as the NRG simulations has been applied, in which specifically the uniformly distributed heat flux at the internal surface of the claddings has been imposed.

Successively, given the effect that the modelling of the rod’s internal electric heater has shown, the complete porous blockage modelling and the related parametric study on porosity and self-

heating have been implemented in the model described in section “4.5.5 Influence of the internal electrical heater modelling”.

The specifications of the setup are summarised in Table 14. Worth mentioning is the fact that the boundary conditions specified below have been implemented with the same approach described in section “4.5.1 Computational domain settings”.

Methods	Standard k-ε (RANS), Turbulent Pr = 2	
Time dependence	Steady state	
Domain	Surface	Boundary condition
Fluid (LBE)	Faces on hexagonal boundary	Translational periodicity boundary condition
	Inlet	$\dot{m}_{in} = 6.54 \text{ kg/s}$ $T_{in} = 200^\circ\text{C}$
	Outlet	p_{out}
Solid (SS 1.4571)	Internal rod surface	$q'' = 0.580 \text{ MW/m}^2$
	Wires and external cladding surface	Conservative interface flux with LBE and blockage
Central blockage	Paste and shell	Conservative interface flux with LBE, claddings and wires

Table 14 – Porous blockage domain model computational setup specification

For sake of clarity, in this chapter the low flow rate case scenario has been represented (see Table 4), to allow in the first place the direct comparison with the results obtained by the sensitivity study done by NRG, as it has been already mentioned. Additionally, it has been decided not to modify such choice for several reasons: first of all, it allows for keeping continuity of the analysis and direct comparison of the results obtained; secondly, due to the general overestimation of the temperatures observed in the previous chapter and therefore a not properly corresponding representation of the experimental phenomena, it is believed that the value of the flow rate implemented is anyhow adequate to give a qualitative explanation of the effect of the porous blockage.

Moreover, for the investigation of the impact of a porous blockage element in a rod fuel bundle, the estimation of the pressure drops across it is needed. The Darcy’s law (Equation 3) is used by the commercial code ANSYS CFX [60] for flows in porous regions:

$$\frac{dP}{dx} = \frac{\mu}{K_p} u_s + K_{loss} \frac{\rho u_s^2}{2} \quad (3)$$

Where $\frac{dP}{dx}$ is the pressure loss per unit length in Pa/m, μ is the dynamic viscosity in Pa·s, u_s is the superficial velocity in m/s, ρ the density of the fluid in kg/m³.

The other two coefficients contributing to the pressure drops are the permeability (K_p , in m²) and the loss coefficient (K_{loss} , in m⁻¹). The former depends only on the geometry of the medium (it is independent of the nature of the fluid) and appears in the linear losses term of the equation, while the latter is an empirical coefficient and appears in the quadratic losses term. [69]

Given the formation process mentioned before, namely accumulation of particles, the most appropriate description of the considered porous blockage is with a packed bed structure, and based on this assumption the two coefficients have been determined. The empirical loss coefficient K_{loss} is considered equal to 800 m⁻¹, established from a simulation of a packed bed structure done in [70]. Besides, according to [69][71], in the case of beds of particles the hydraulic radius theory of Carman-Kozeny can be introduced, leading to the following expression for the permeability:

$$K_p = \frac{d^2 \varphi^3}{36(1-\varphi)^2 K_k} \quad (4)$$

Where d is the particle diameter, for a bed made of uniformly sized spheres, and φ is the porosity. The coefficient K_k is the Kozeny constant defined as $K_k = K_0 \tau^2$: K_0 is a shape factor normally equal to 2.5 and τ is the tortuosity approximated by $2^{1/2}$ for packed beds of spheres. [71]

The Carman-Kozeny equation gives satisfactory results for media that consist of particles of approximately spherical shape and whose diameters fall within a narrow range. [69][71] Since in the present thesis also self-heating of the blockage is considered, hence assuming that it is originated by the accumulation of fuel material released after a pin disruption, the diameter of the particles is taken from a study done on the modelling of fuel fragmentation and particle size distribution in fragmented fuel, being it equal to 1.4 mm [72].

As far as the porosity is concerned, it is defined as the local ratio of the volume of fluid to the total physical volume [60] and is determined by the size and shape of the particular matter [73]. In the few publications investigating the effect of porosity in partially blocked bundles [72][73][74], both heat transfer experiments and numerical evaluations applied mostly to sodium loops have used values of porosity ranging between 0.3-0.4. In the present analysis a parametric study on the porosity value has been done, varying the parameter in the specified interval.

In conclusion to this chapter also an evaluation of the impact of self-heating of the blockage has been done, postulating that the origin of the blockage could be an accumulation of fuel particles after fuel failure, therefore the power that such obstruction would have is equal to the heat produced by one fuel pin in normal operating conditions. Consequently, in the model a volumetric heat source has been added to the porous blockage in order to simulate the heat release. Also in this case scenario a parametric study has been done on the generated power level with fixed porosity ($\phi=0.4$).

In the following subsections the results of the analysis will be presented, with a qualitative explanation of the influence of porosity and self-heating on the temperatures in the 19-pin wire wrapped fuel bundle modelled.

5.1.1 Blockage with porous shell

In this section the results of the model in which the central blockage casing has been defined as a porous medium are presented. The case scenario investigated is the one mentioned in the previous paragraphs, in which specifically a porosity of 0.5 has been imposed.

The initial idea behind the modelling of the porous shell has been to imitate the work done by NRG [46], in which they investigated the eventual presence of leakage paths between the blockage casing and the rods by replacing the steel material of the blockage casings is replaced by liquid LBE. Thanks to the setup settings chosen, the direct comparison with those results, as well as with the experimental campaign data for the low mass flow rate case scenario can be done.

Figure 56 and Figure 57 show respectively the effect of the porous shell with respect to the steel one, and the impact of a porous gap with respect to a liquid one. As expected, in the figure below, one can notice the decrease in the temperature value at all the TCs positions. This is not surprising, since liquid LBE is now allowed to flow, even if in a limited extent, thus it cools down slightly the cladding surface. The temperatures appear to be lower also at the level of the unblocked TCs, probably because the lower degradation of the heat transfer due to the presence of some porosity leads to an overall lower heating of the coolant.

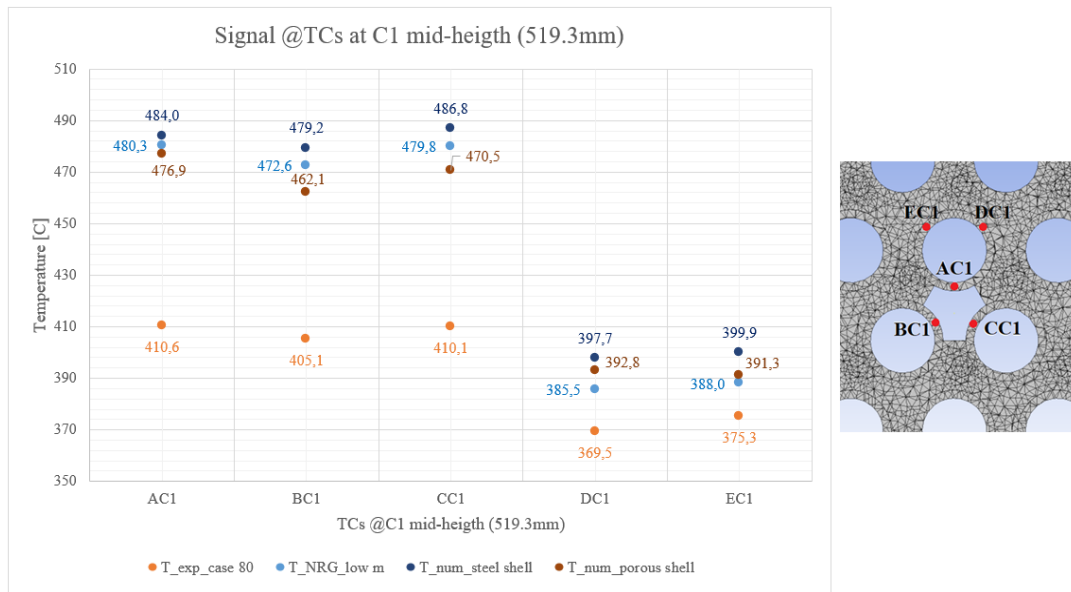


Figure 56 – Effect of the porous shell on the temperature value at the blockage mid-height in the refined blockage domain

Likewise, the scope of the figure below has been to simulate the eventual leakages that could be present at the interface between the cladding and the steel shell, since perfect contact couldn't be guaranteed by the blockage installation procedure within the experimental rod bundle. It is indeed clear that compared to a full liquid gap, where the cold LBE can flow in the space between the walls and cool down the cladding surface where the TCs are present, the allowed degree of porosity leads generally to higher temperatures.

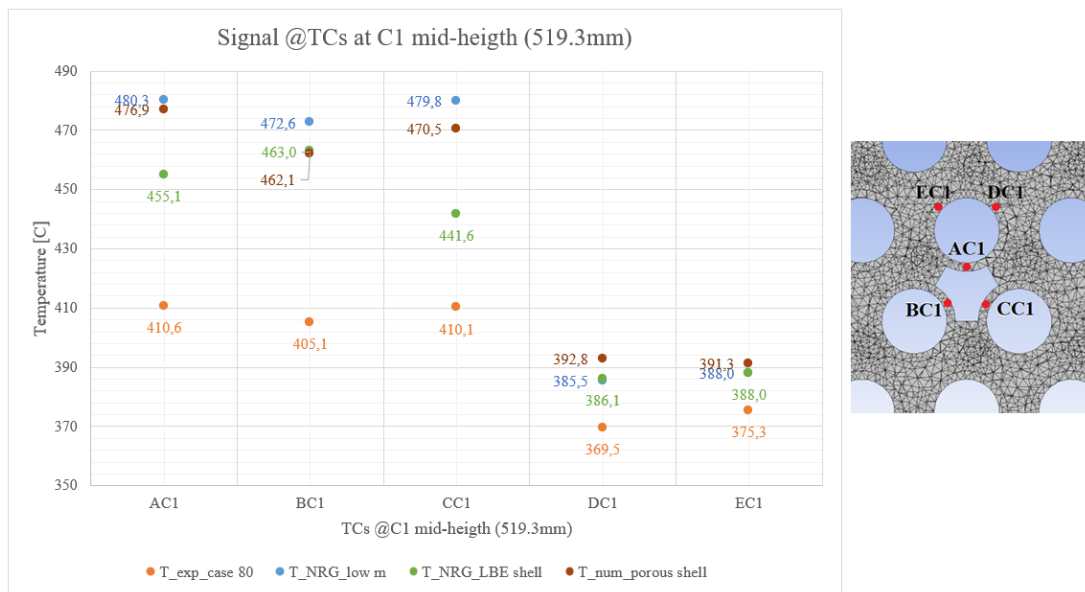


Figure 57 – Comparison of the temperature value between the porous shell and LBE leakage path at the blockage mid-height in the refined blockage domain

Figure 58 represents the axial velocity profile comparison between the case with the porous and with the steel shell. Obviously, since the velocities are sampled on the line crossing the centre of the blockage (yellow line in Figure 39), one can see that non-zero velocities are present where now the porosity is allowed, since LBE can flow (black arrows in Figure 58), whereas, opposingly, the core of the blockage is still solid so the velocity results null. The recirculation zone in the wake of the blockage appears to be less impacted, probably because the possibility of flow around the blockage paste results in a less disturbed flow, compared to a complete obstruction.

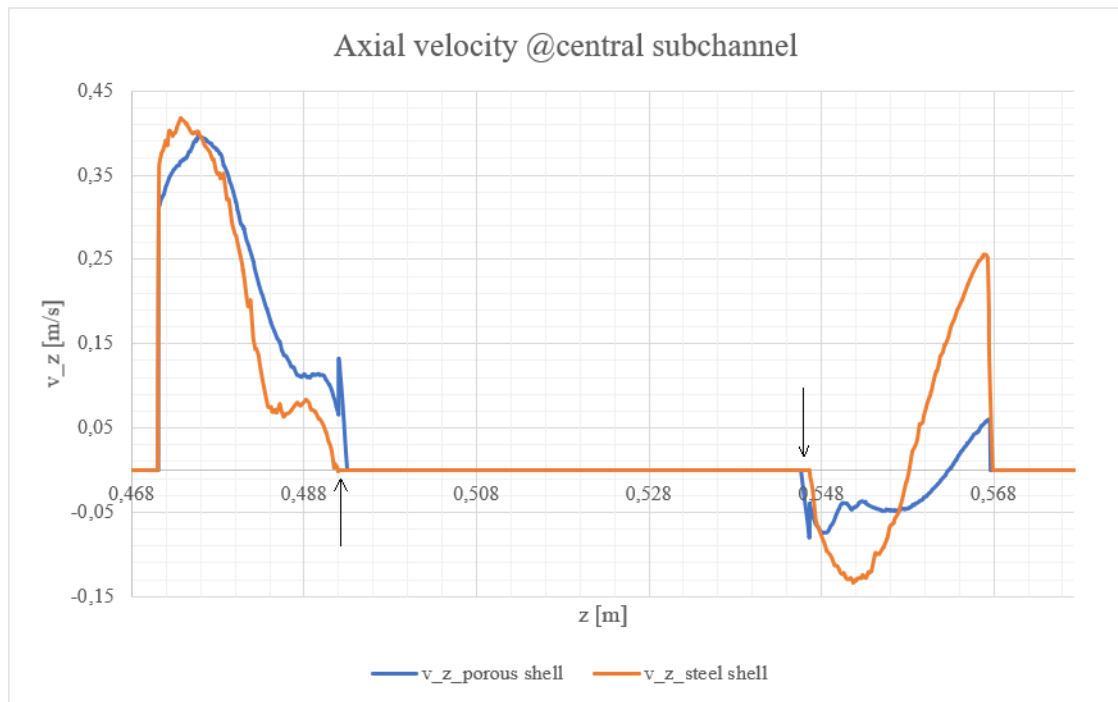


Figure 58 – Effect of the porous shell on the velocity profile along the line at the centre of the blocked subchannel in the refined blockage domain

The temperature profiles depicted in Figure 59 are sampled on the same line as before. Here it is possible to see that even if the steel is a well conducting material, the presence of the porosity allowing for LBE flow has a bigger effect on the temperatures. Indeed, these increase with a slower rate, represented by the shift in the profile just upstream the paste element, leading to a lower heating up inside the low conducting paste material. It is supposed that the higher temperatures downstream the blockage paste are due to the contribution of the LBE that have been flowing around it, therefore hotter compared to the coolant flow coming from the adjacent subchannels.

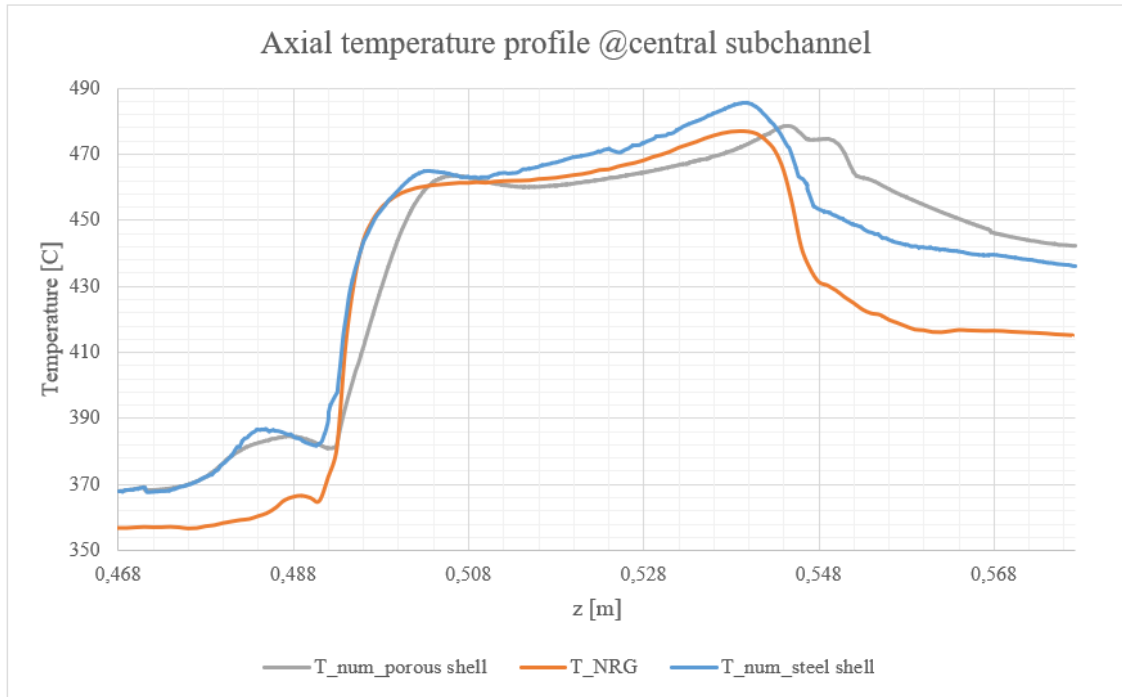


Figure 59 – Effect of the porous shell on the temperature profile along the line at the centre of the blocked subchannel in the refined blockage domain

In conclusion to this section, the temperature distribution at the blockage mid-height is depicted in Figure 60 for the two cases compared: steel and porous shell. As already explained, it confirms that in presence of a certain degree of porosity the temperatures are locally lower, since the flow of relatively cold LBE allows for some cooling of the surfaces, even if in a limited extent.

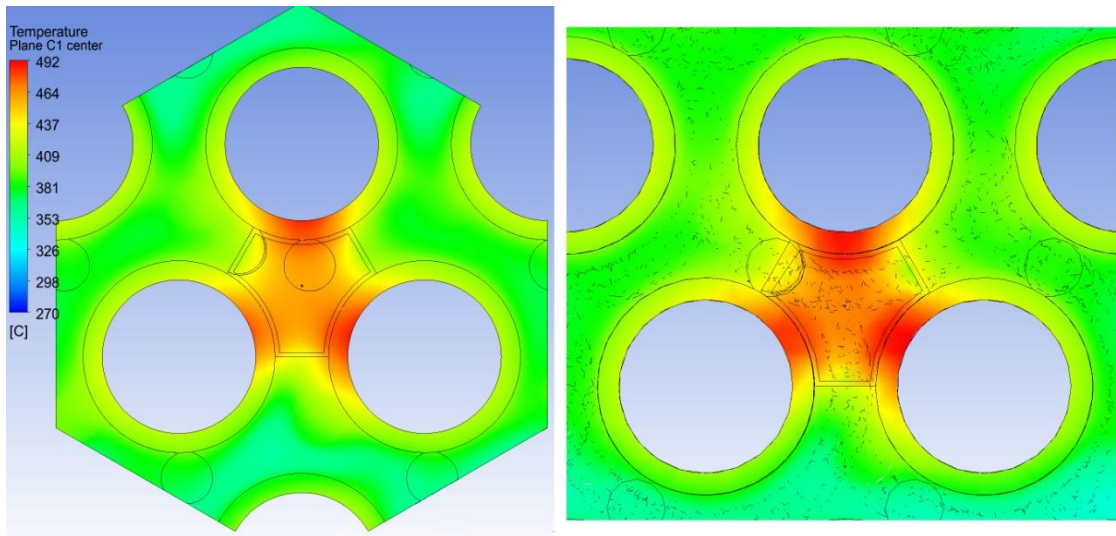


Figure 60 – Comparison of the temperature distribution at the cross-section of the blockage mid-height between the porous shell (left) and steel shell (right)

5.1.2 Porous blockage

In this section the results of the model in which the central blockage has been defined as a complete porous medium are presented. At first, the case scenario in which the imposed porosity is equal to 0.4 is investigated, and successively the results of the parametric study on the value of the porosity are showed.

Figure 61 depicts the comparison between the temperatures evaluated at the TCs present at the blockage mid-height for the different case scenarios analysed so far: solid blockage and porous blockage. As expected, the implementation of a full porous obstruction leads to lower temperatures at the cladding surface where the TCs are embedded. Such difference is majorly observed at the TCs facing the blockage, at which the maximum temperature difference encountered is of 25K. The lower difference measured at the unblocked TCs is thought to be accounted to the general lower temperature of the coolant, since the heat transfer is less degraded compared to the case with the solid blockage, because albeit the partial obstruction the coolant flow is allowed in the blocked region.

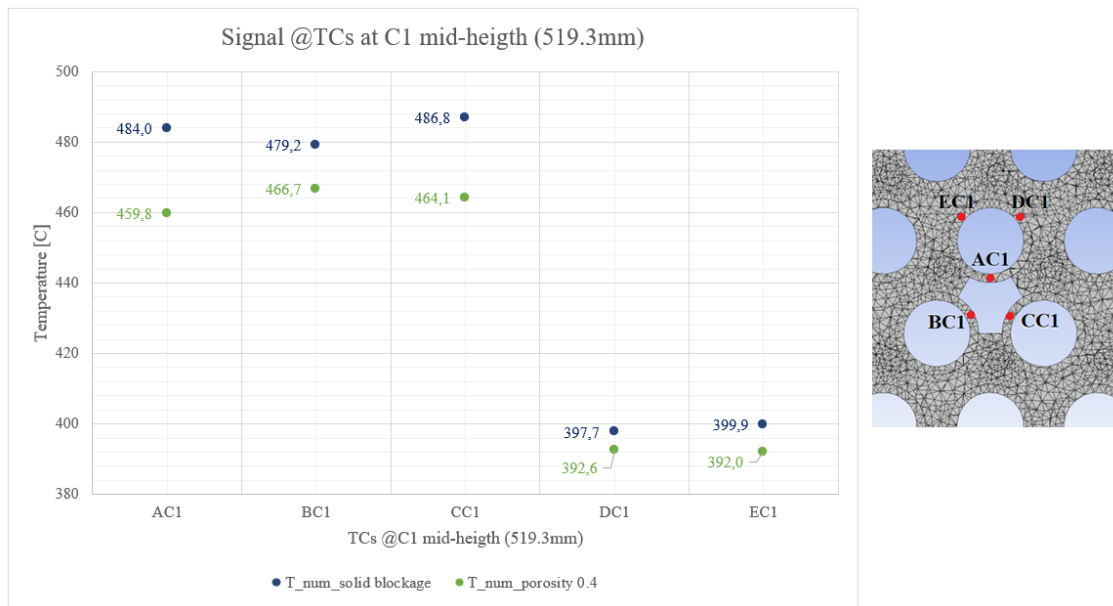


Figure 61 – Comparison of the temperature value between the porous and solid blockage at the blockage mid-height in the refined blockage domain

Figure 62 and Figure 63 show respectively the velocity and temperature profiles evaluated along stream-wise line passing through the centre of the blocked subchannel (yellow line in Figure 39). In the first mentioned plot, it is possible to identify the axial velocity comparison between the solid and the porous blockage. It is clear that some flow disturbance is present just upstream and

downstream the obstruction, as it has been observed for the solid blockage as well, but with a smaller intensity. This is because the coolant is allowed to flow, although in a limited manner. The visible discontinuity present is where the coolant enters the porous blockage: it is supposed that the steep increase in velocity is caused because the LBE is now flowing in the much more narrower pores of the blockage. One can see also that the velocity decreases gradually the more the coolant flows inside the element, until at some locations it reaches stagnation.

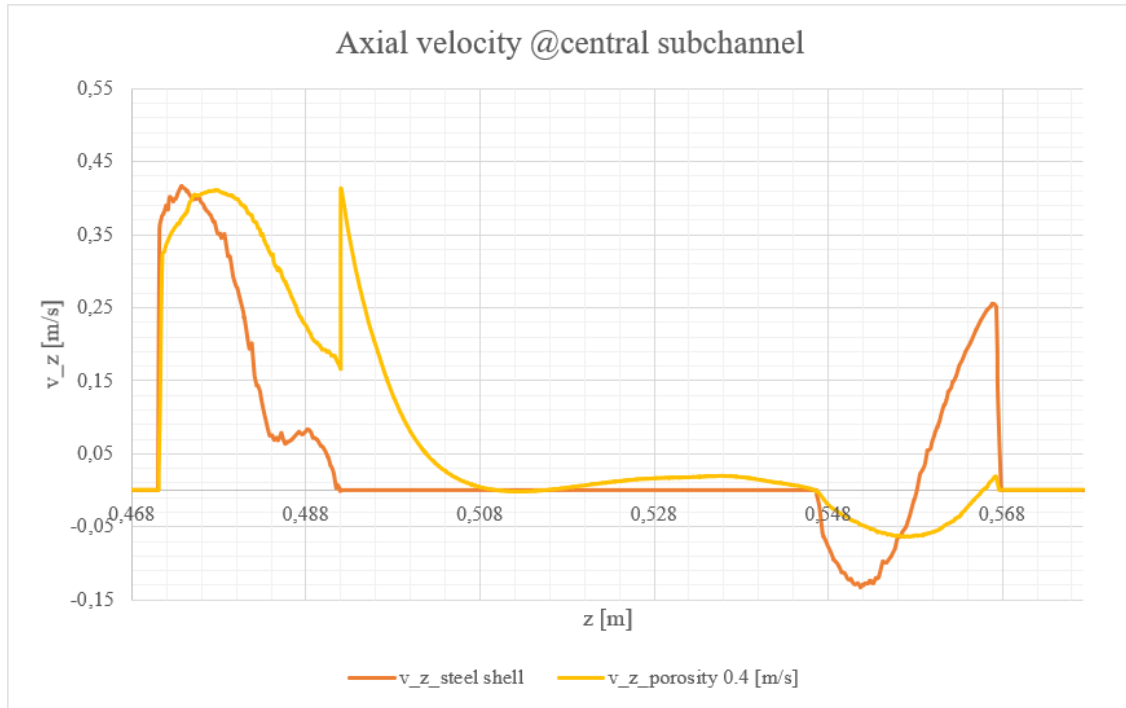


Figure 62 – Effect of the porous blockage on the velocity profile along the line at the centre of the blocked subchannel in the refined blockage domain

Evidently, the behaviour of the velocity just explained has an impact on the temperature profile visible in Figure 63. Indeed, the initially faster flow of the LBE leads to a lower and slower warming of the first obstructed section, visible by the shift in the curve compared to the solid blockage case. On the contrary, the two peaks are confirming that as soon as the coolant is stagnant, the temperature rises significantly, to decrease again when the flow is allowed.

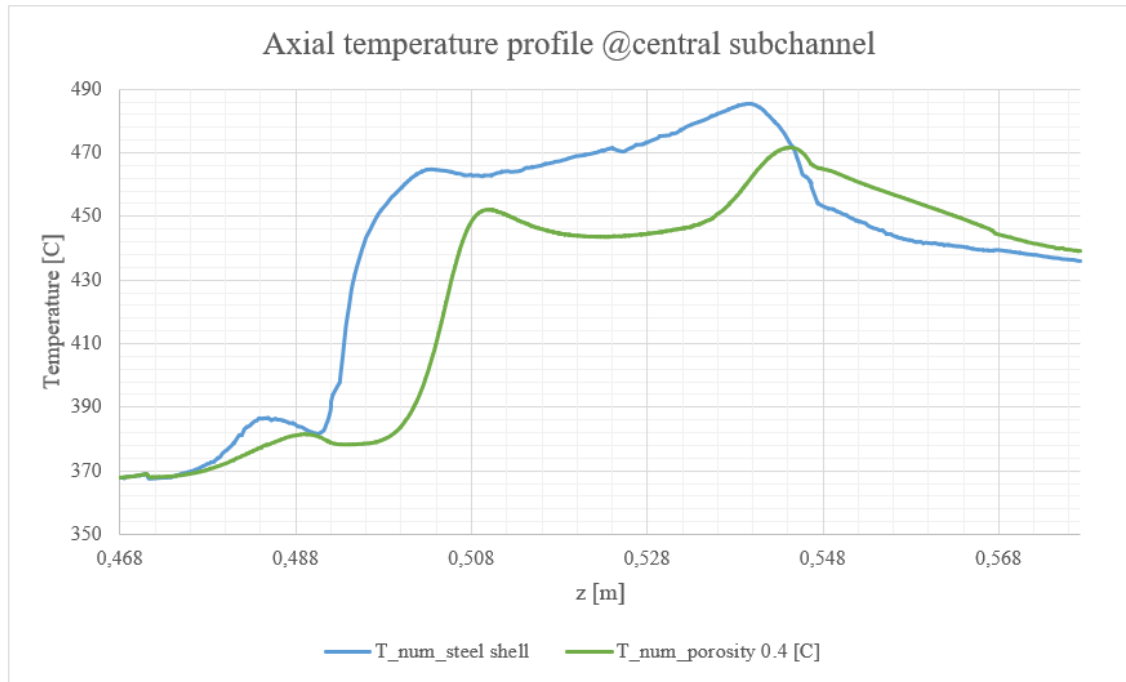


Figure 63 – Effect of the porous blockage on the temperature profile along the line at the centre of the blocked subchannel in the refined blockage domain

Besides, this observation is reinforced by the velocity and temperature distribution plotted in Figure 64 along a plane parallel to the flow direction crossing the centre of the porous blockage. The coolant flow is from right to left. Additionally, also the thermohydraulic flow field evolution along the fuel bundle is represented in Figure 65, where the displayed cross-sectional planes are placed at the bottom, at the centre and at the top of the porous blockage. From these plots one can notice that the maximum temperature is located towards the end of the blockage, and in general the higher temperatures are obviously reached where the velocity of the LBE is lower. The former observation could also be related to the asymmetric axial heat transfer caused by the hotter wake region compared to the colder region upstream the blockage. In the wake of the porous blockage the temperature slightly decreases thanks to the contribution of the relatively colder coolant from the adjacent subchannels. Indeed, it is possible to notice that within the bundle higher temperatures are prevailing at the inner sub-channels and lower at the outer ones.

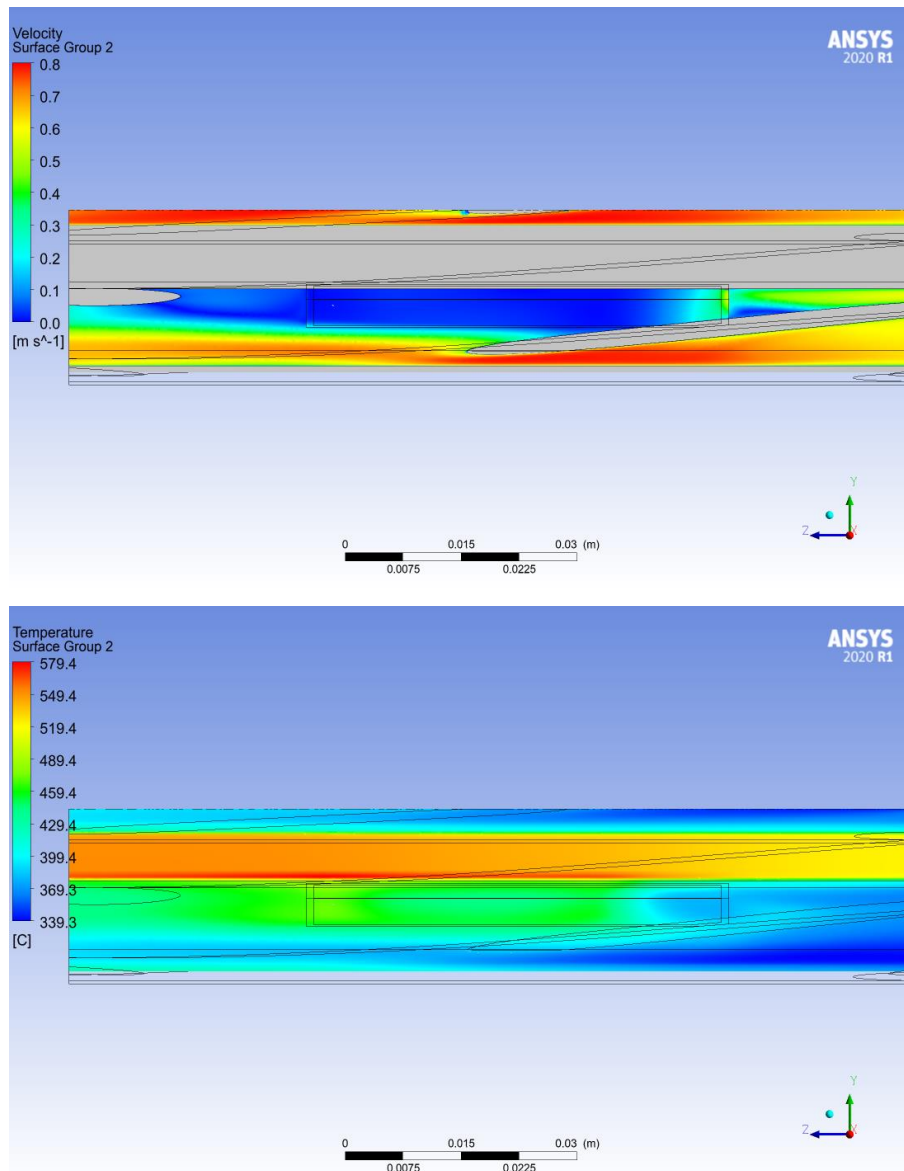


Figure 64 – Velocity (above) and temperature (below) distribution along a plane parallel to the flow direction crossing the centre of the porous blockage

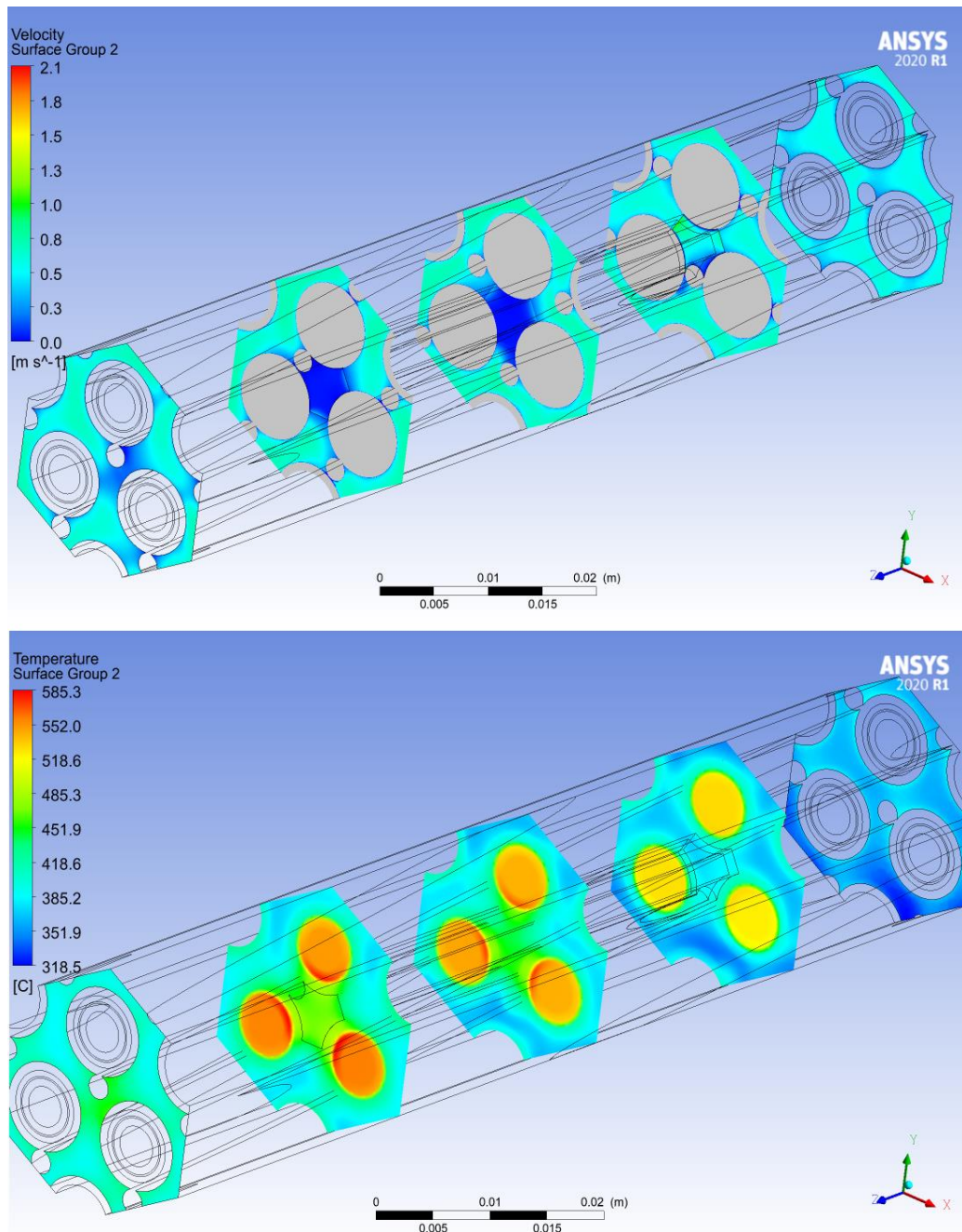


Figure 65 – Velocity (above) and temperature (below) evolution along the fuel bundle

Proceeding further with the analysis, it has been mentioned at the beginning of this chapter that a parametric study on the porosity value has been done, varying the parameter in the range between 0.3-0.4. Here below the comparison of the results obtained will be represented, as function of the porosity, in order to investigate to which extent does this parameter affect the quantities investigated.

First of all, Figure 66 shows the comparison between the axial velocity profile along the stream-wise line passing through the centre of the blocked subchannel (yellow line in Figure 39). A further comment can be added to the observations described above: as expected, the value of the velocity peak increases with decreasing porosity, because the pores of the obstructing object are smaller, therefore the velocity of the LBE increases.

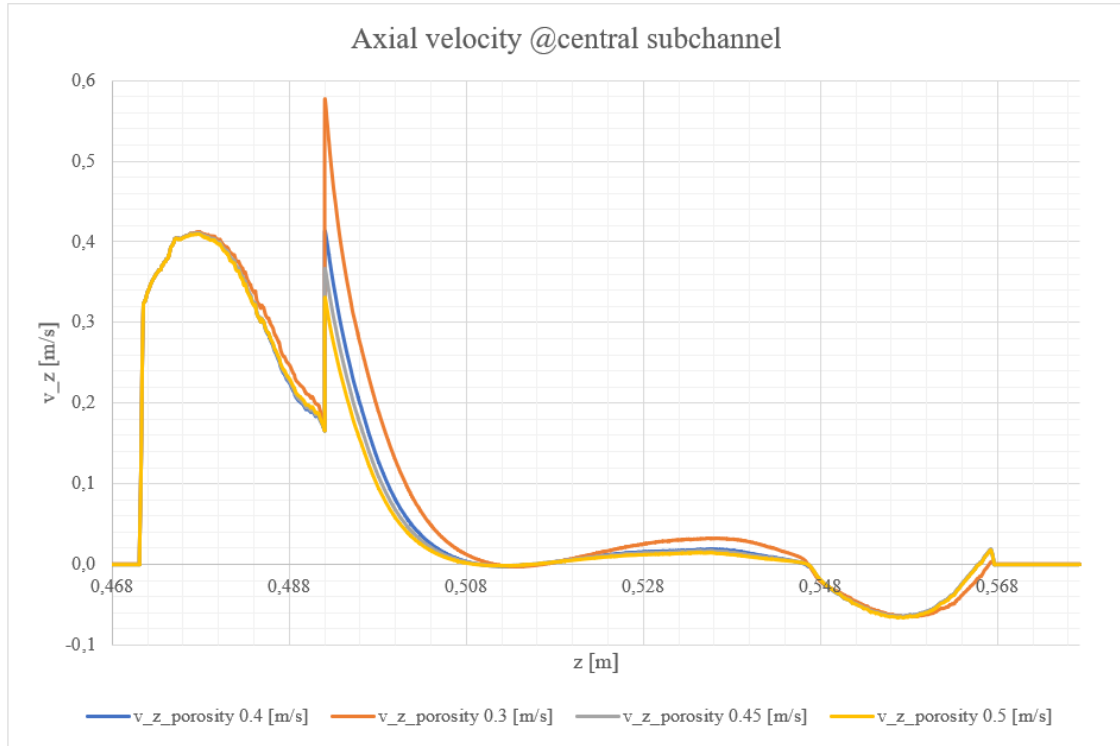


Figure 66 – Effect of the porosity on the velocity profile along the line at the centre of the blocked subchannel in the refined blockage domain

In Figure 67 are shown the maximum temperatures in the LBE, in the porous blockage and at the cladding surface corresponding to the contact area with the blockage as function of the porosity. One can see that the effect of the porosity change on the maximum temperature is only marginal, mostly if the porous blockage and the cladding surface are considered. Indeed, they all show a quite constant behaviour. On the contrary, even if slightly, the maximum temperature of the coolant increases with decreasing porosity, not surprising fact since the flow inside the obstruction is more limited. It is supposed that such tendency will be kept if the porosity would be decreased further.

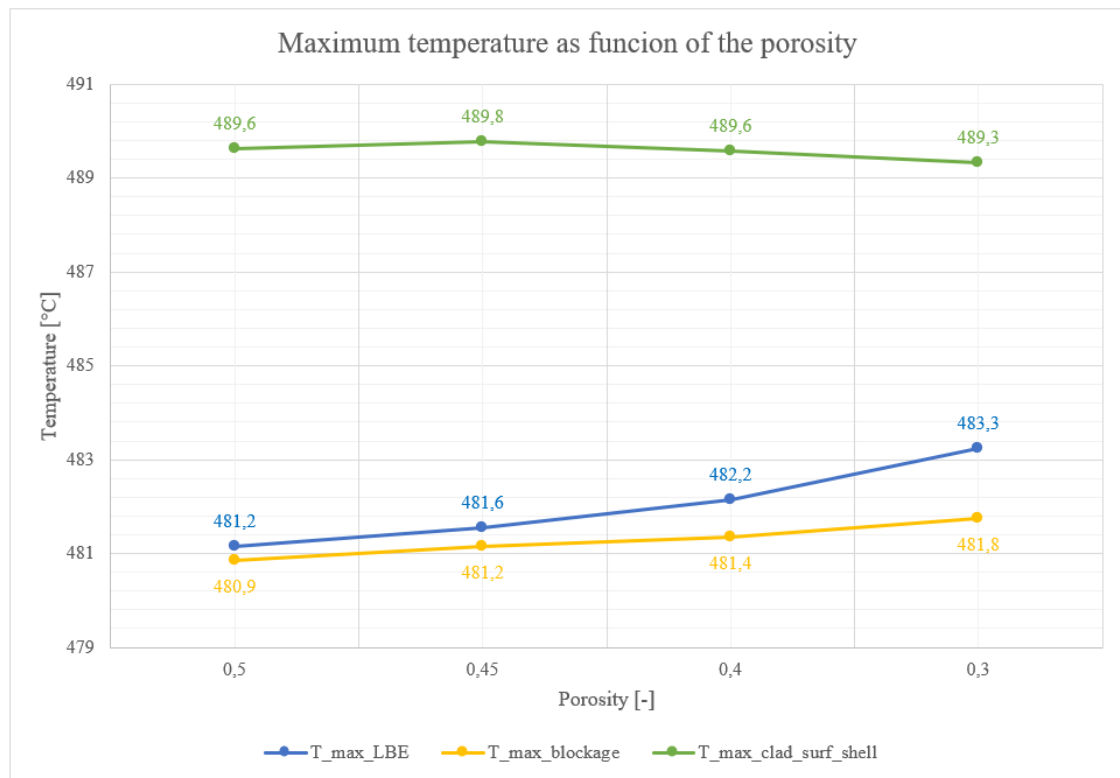


Figure 67 – Maximum temperatures in the LBE, in the porous blockage and at the cladding surface as function of the porosity

On the other hand, the temperature profile along the axial direction depicted in Figure 68 for every value of porosity goes completely in opposition to the trend just described above: beside the fact that the overall behaviour described above is confirmed, the values of the temperatures inside the porous blockage are decreasing with the porosity. It is supposed it could be explained by the fact that due to the smaller flow of coolant inside the porous blockage, necessarily it has to increase in the surrounding subchannels, therefore contributing to a higher cooling of such obstruction.

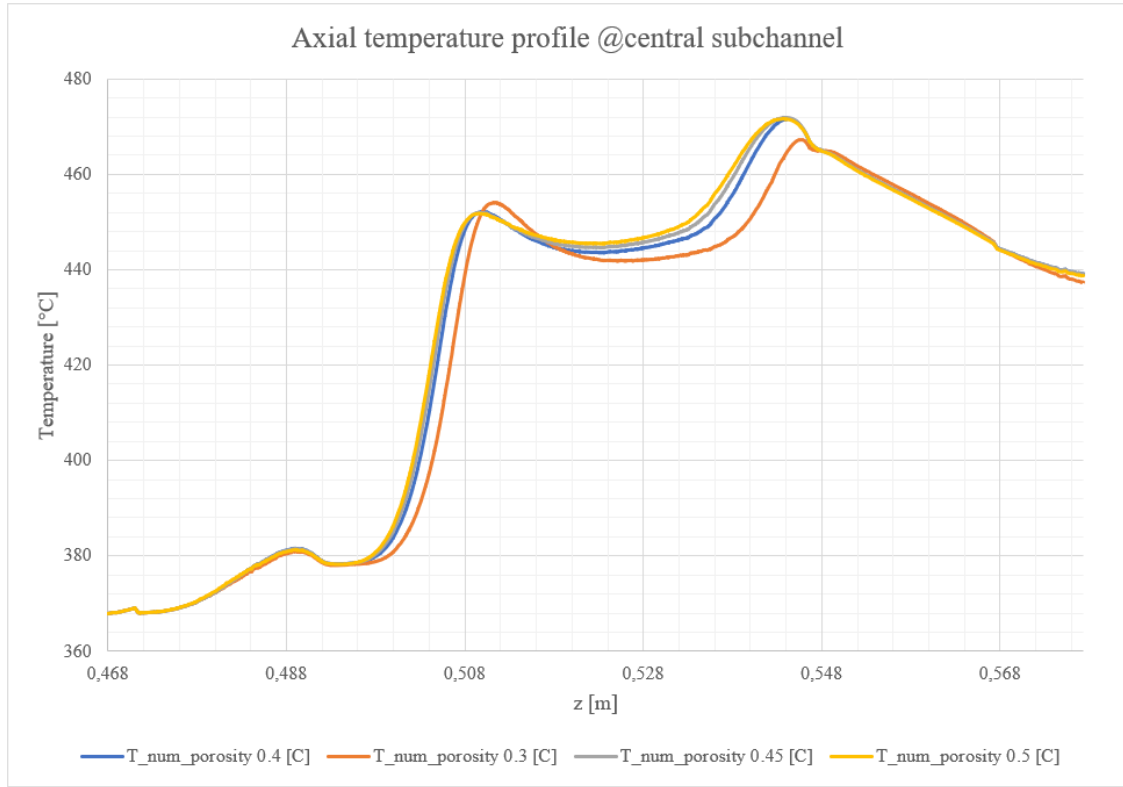


Figure 68 – Effect of the porosity on the temperature profile along the line at the centre of the blocked subchannel in the refined blockage domain

To conclude this section, it is important to mention that the pressure drop across the porous blockage evaluated for all the cases is in the range of 1.3 kPa and the effect of the change of porosity can be neglected. This could be explained by the fact that the blockage has relatively small dimensions and that the range of values of porosity is narrow, hence no big difference between the cases is expected.

5.1.3 Porous blockage with self-heating

In the same fashion as it has been done in the previous section, here the results of the model with the self-heated porous blockage are presented, since it has been assumed that the origin of the blockage could be an accumulation of fuel particles after fuel failure. Therefore, with a constant porosity of 0.4, the power produced by the blockage has been imposed equal to the heat produced by one fuel pin in normal operating conditions. Moreover, later in this section the results of the parametric study on the generated power level are showed.

Figure 69 depicts the comparison between the temperatures evaluated at the TCs present at the blockage mid-height for the different case scenarios analysed: porous blockage with fixed porosity, with and without self-heating, from now on referred as hot and cold porous blockage

respectively. As expected, the implementation of power generation inside the porous obstruction leads to much higher temperatures at the cladding surface where the TCs are embedded, principally at the ones facing the blockage, at which the maximum temperature difference encountered is of 130K. Inversely, the temperatures at the unblocked TCs are poorly affected, since they are facing the undisturbed and relatively cold coolant.

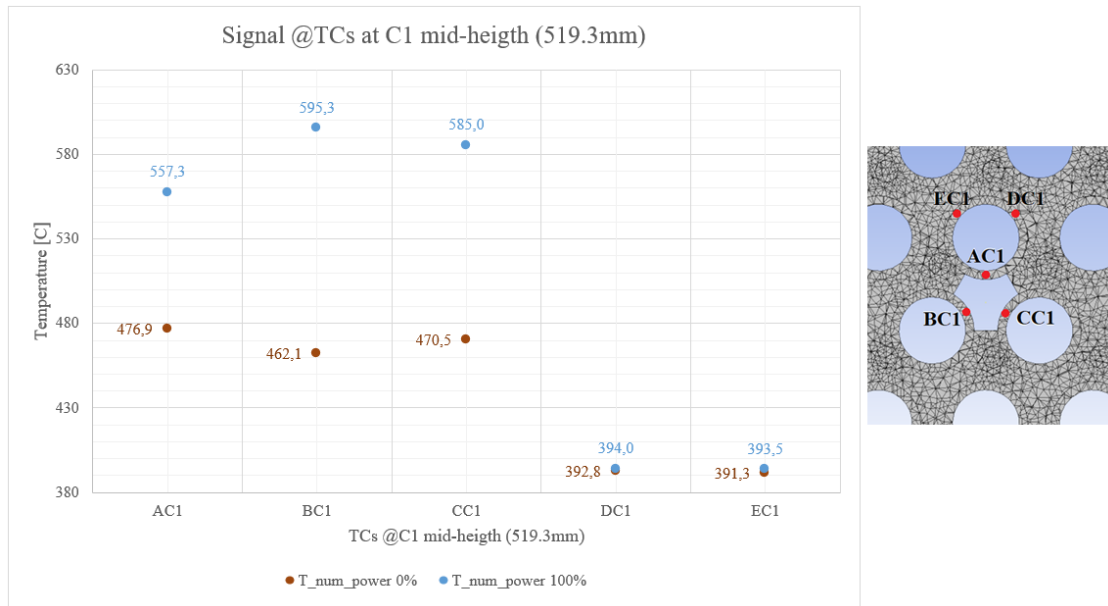


Figure 69 – Comparison of the temperature value between the full and no self-heating of the porous blockage at the blockage mid-height in the refined blockage domain

It is important to mention that since the value of the porosity has not been changed, all the observations explained in section “5.1.2 Porous blockage” regarding the hydraulic field is still valid. Indeed, the velocity and the pressure drop are unvaried.

Nonetheless, the temperatures are clearly affected, as shown in Figure 70, which is representing the comparison of the two temperature profiles evaluated along stream-wise line passing through the centre of the blocked subchannel (yellow line in Figure 39). Obviously, one can notice that the temperatures are much higher in magnitude and the behaviour mentioned in section “5.1.2 Porous blockage” are highly accentuated, when the power is present, since the heat released is much greater. In addition, the decrease in temperatures in the wake of the hot porous blockage is supposed to be due to the cooling contribution of the relatively cold coolant from the adjacent subchannels.

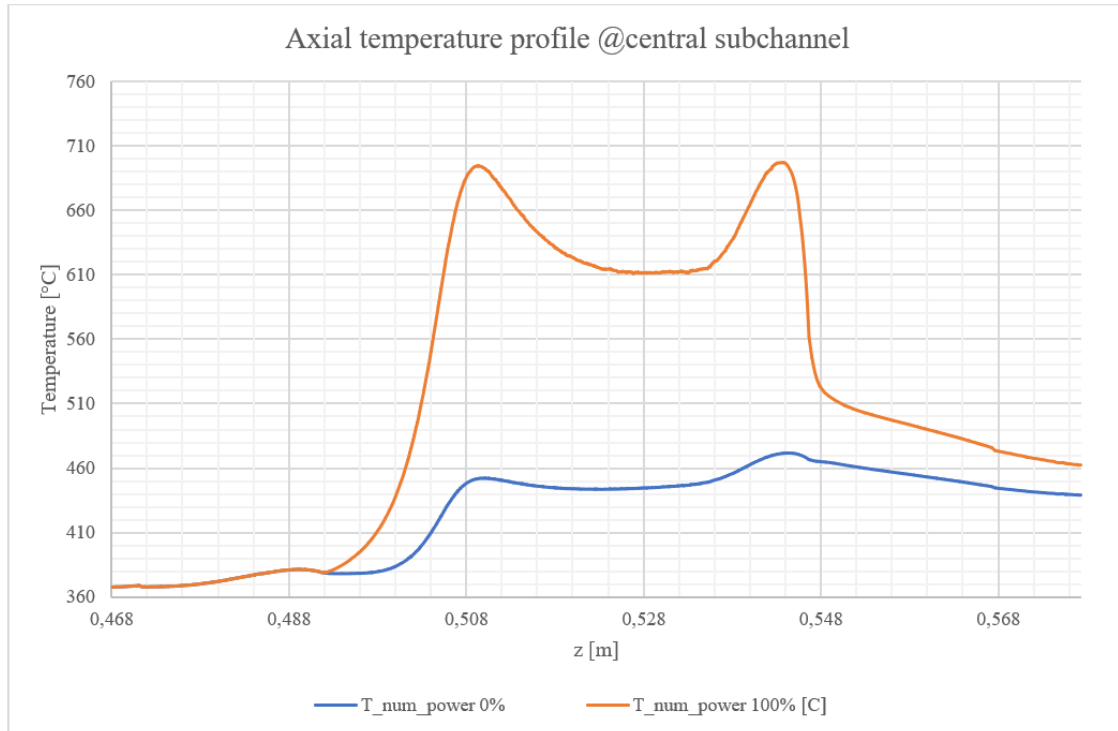


Figure 70 – Effect of the self-heating of the porous blockage on the temperature profile along the line at the centre of the blocked subchannel in the refined blockage domain

For a better understanding of the occurring phenomena just described, Figure 71 shows the temperature distribution plotted along the plane parallel to the flow direction crossing the centre of the porous blockage (the coolant flow is from right to left), and the temperature field evolution along the fuel bundle, where the displayed cross-sectional planes are placed at the bottom, at the centre and at the top of the porous blockage. From these plots one can clearly locate the peaks identified in the figure above.

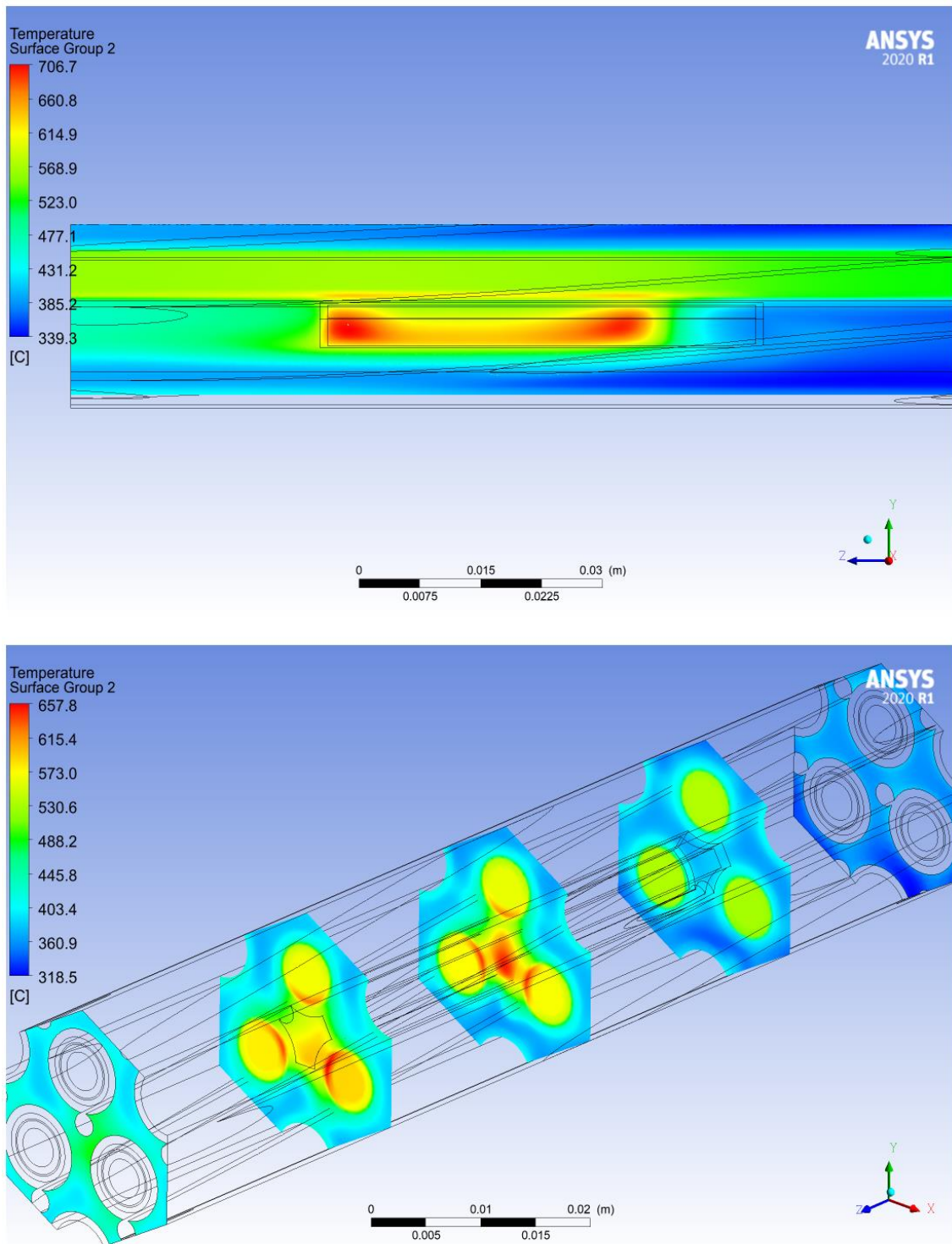


Figure 71 – Temperature distribution along a plane parallel to the flow direction crossing the centre of the porous blockage (above), temperature evolution along the fuel bundle (below) for the case scenario with hot porous blockage

Proceeding further with the analysis, it has been mentioned at the beginning of this chapter that a parametric study on the generated power level has been done, varying the parameter from 10% to full power conditions. Here below the comparison of the results obtained will be represented, as function of the power, in order to investigate to which extent does this parameter affect the quantities investigated.

In Figure 72 are shown the maximum temperatures in the LBE, in the porous blockage and at the cladding surface corresponding to the contact area with the blockage as function of the generated power level. As expected, one can see clearly that the temperatures are steadily increasing with increasing power generated inside the hot porous blockage. For this reason, it should be of no surprise that the maximum temperatures measured in the obstruction are higher with respect to the ones at the cladding surface, since the power generated in the latter is locally lower and the steel material is better heat conducting.

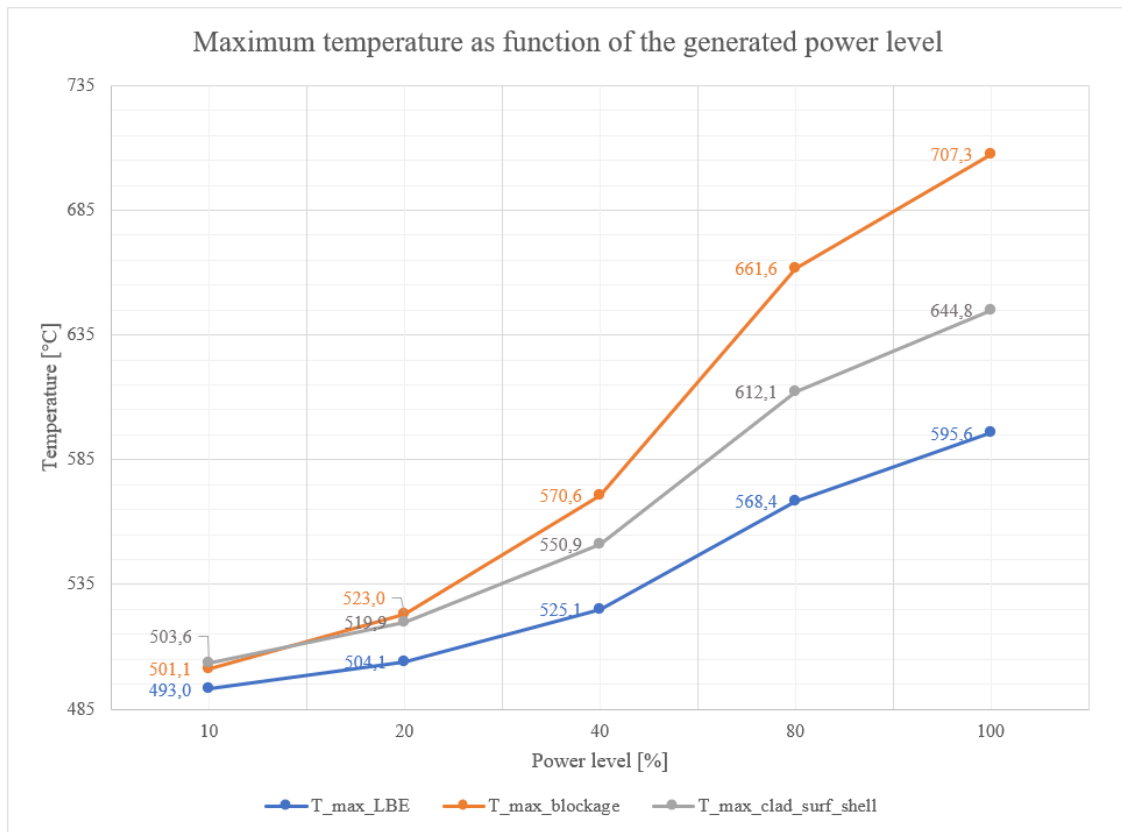


Figure 72 – Maximum temperatures in the LBE, in the hot porous blockage and at the cladding surface as function of the generated power level

Finally, the temperature profile along the axial direction depicted in Figure 73 for every value of the generated power level is in agreement to the trend just described above: besides the fact that

the overall behaviour described above is confirmed, one can visualise once again that the increase in the power generated by the hot porous blockage is enhancing the effects described.

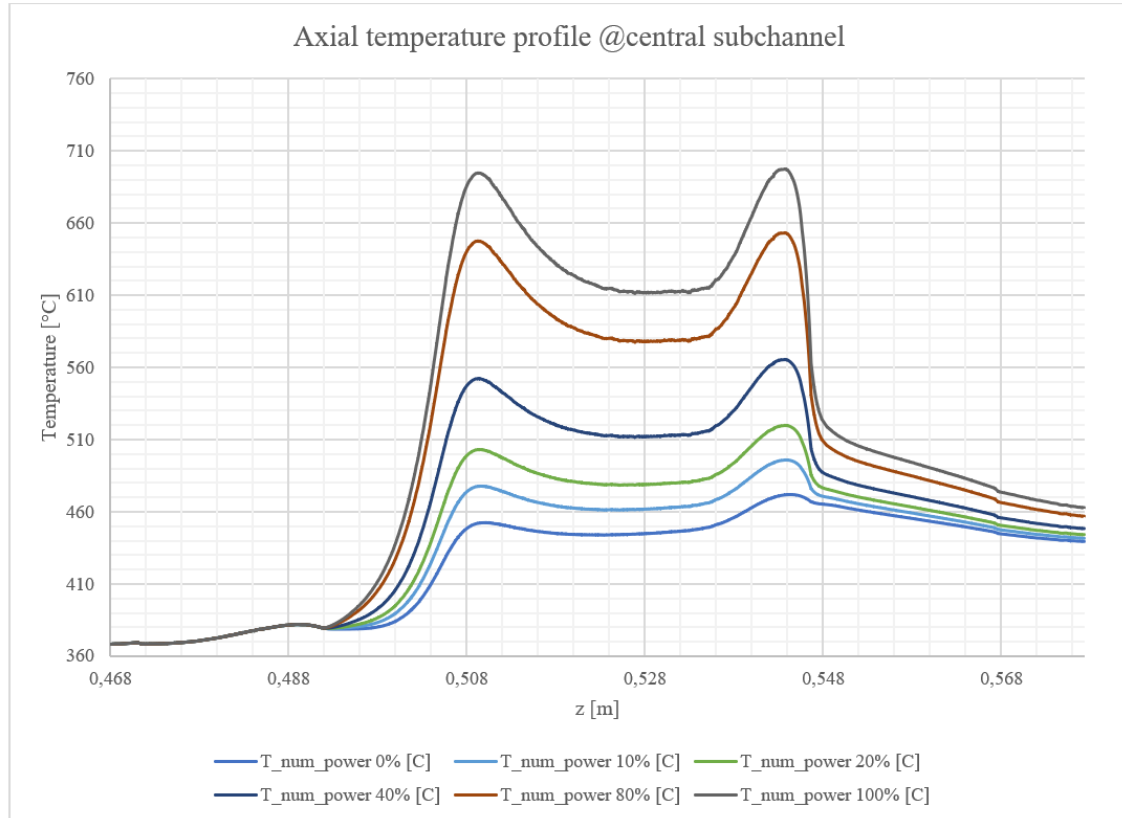


Figure 73 – Effect of the generated power level in the porous blockage on the temperature profile along the line at the centre of the blocked subchannel in the refined blockage domain

5.2 Conclusions

In the current chapter the analysis has been focused on the presence of a porous blockage in the lead-cooled 19-pin wire-wrapped fuel bundle. At first, only the blockage casing has been modelled as a porous material, then the complete porous blockage has been implemented, to conclude with the addition of its self-heating. To reach a better understanding of the phenomena involved, a parametric study on the porosity and the generated power level has been performed.

As it has been done already before, the procedure used has been explained, presenting the details of the assumptions made, the geometry and mesh used, as well as the computational setup has been described. It is important to mention that the aim of this chapter has been to give a qualitative explanation of the effect of porosity and self-heating on the parameters under investigation, since the model used presents some issues in the quantitative prediction of the temperatures in the blocked domain section, as it has been already discussed in “Chapter 4 – Fuel assembly model

with solid blockage”. For this reason, it has not been possible to make a specific safety assessment of these potential accidental scenarios.

Nevertheless, the results obtained show that compared to a solid blockage, the implemented degree of porosity leads to lower temperatures at the cladding surface where the TCs are embedded, since even if limited, the flow of coolant is allowed to a certain extent. For this reason, where the fluid is stagnant, the temperature rises significantly again and the maximum temperature is located towards the end of the blockage. Although the overall behaviour described is observed for all the porosities simulated, the maximum temperatures are affected only marginally by the change of porosity. On the other hand, the influence of the porosity can be seen by the temperature profiles along a stream-wise line at the centre of the blocked subchannel: the values of the temperatures inside the porous blockage are decreasing with the porosity. It is supposed it could be ascribed to a higher cooling from the LBE flowing from the adjacent subchannels.

As far as the self-heating is concerned, it has been applied in order to simulate the potential blockage generation through accumulation of fuel particles. Considering a constant value for the porosity, the effect of the internally generated power is clearly the substantial increase in the temperatures in the blocked region. The maximum temperature has two peaks: one always towards the end and the other just upstream the centre of the blockage. These are the locations where the fluid is stagnant, and the power generated heightens the warming at those locations. Besides, the impact of the change in the generated power level agrees with this latter conclusion: the always visible overall behaviour of the temperatures is enhanced with increasing power, and the maximum temperature steadily increase while going to full power conditions. It is important to mention that despite the temperature shoot up in case of these active local blockages might be excessive and lead to pin failure, their presence is detected rapidly thanks to the delayed neutron detection signal, as mentioned in [74]. This is instead not so easy for local cold blockages: their detection through changes in the reactivity in the reactor is not immediate, in addition to the fact that the pressure drop across them is limited and the overall mass flow rate is marginally affected, therefore the outlet flow conditions don't change sufficiently to allow for a prompt presence determination. Yet, in the eventual case that the occurring local hot spots lead to pin cladding failure, the fuel leakages can be detected by the fission gas release.

Ultimately, although the local blockage detection is of paramount importance in order to avoid the initiation of accidental scenarios and propagation of core damage, it is relevant to highlight

that, even in the range of temperatures obtained in the analysed worst case scenario (high power generation and low mass flow rate), the criterion of core damage propagation is unlikely to be met. In fact, according to the cladding burst criterion, cladding failure in a short-term transient is expected above $\approx 930^{\circ}\text{C}$. It is true that creep effects start to have an impact on the long term above $\approx 550^{\circ}\text{C}$ and that higher the temperature, the faster the occurrence of failure; nevertheless, even if local blockages are not immediately detected, the creep effect would not be important yet.

To conclude, since local porous blockages in LBE-cooled rod bundles with wires spacers are more likely to appear and that the current safety scenarios should include the hypothetical accidents initiated by the formation of accumulation of particles, either with self-heating or not, it is recommended the simulation of porous blockages in the complete 19-pin wire-wrapped fuel bundle domain, in order to investigate precisely the flow recovery. It is nevertheless believed that this will occur faster compared to the situation with a solid blockage in the same conditions. Moreover, the effect of porosity and self-heating should be evaluated in the high flow rate case scenario, in order to confirm the observations made in this thesis, and to confirm the small sensitivity of the maximum temperature with the porosity.

Conclusions and perspectives

The thermohydraulic flow field within a 19-pin wire-wrapped fuel bundle in presence of an internal blockage has been predicted for the safety assessment of the MYRRHA reactor by CFD simulations. The simulations covered three main case scenarios: unblocked fuel bundle, central solid blockage obstructing one central subchannel and porous blockage, both heat-generating and non-heat-generating.

For the first two studies mentioned, in order to validate the models, the results have been compared with the data obtained from the experimental campaigns within the European projects SEARCH and MAXSIMA respectively, which have been both conducted in the test facility at KIT [45]. In addition, the comparison with the previous numerical analyses performed by NRG has been done as well, after which it has been considered relevant to investigate the origin of the observed big temperature difference between the numerical results and the experimental data.

Several parametric studies have been therefore performed, in which the influence of buoyancy, thermocouple position, turbulence model, mesh refinement and conduction in the electrical heater has been investigated. One should mention that a reduced and refined computational domain centred around the blockage has been modelled, in order to specifically address in detail some of the studies mentioned. Unfortunately, only the inclusion of the electrical heater in the CFD simulation has showed a higher impact on the temperatures measured at the TCs.

The third case scenario analysed is the one including the porous blockage, at first considered cold, to then evaluate also the possibility of eventual self-heating. After having investigated in which extent the porosity and the self-heating were affecting the results, the conclusions that can be drawn are that generally, although the model shows a decrease in temperatures compared to the solid blockage, changing the porosity little sensitivity is observed in the maximum temperature. On the contrary, the temperatures in the model are much more affected by the presence of heat generation in the porous obstacle, where in general they increase with increasing power level. Unfortunately, due to the aforementioned encountered difficulties in the proper prediction of the physical phenomena, it has been possible only to make a qualitative evaluation of the effects on the parameters of interest, and therefore no safety limits have been taken into account.

It is clear that the wire-wrapped rod bundle is a complex geometry to build and to model in CFD. These complexities, both in the experimental construction of the test section and in the numerical implementation of the problem, are causing inevitable uncertainties, that are eventually leading to discrepancies in the results obtained, rendering difficult the validation of numerical models.

Though, it is important to mention that these difficulties are linked to the demanding design specifications and to the advanced technology of this innovative project, yet the feasibility of the installation is not under questioning. On the contrary, it is relevant to analyse thoroughly with representative mock-ups and numerical simulations how the system works, in order to obtain and build a safe and efficient installation.

Hence, it is of paramount importance to understand and to explain the gap between the experimental and numerical values observed. For this reason, as far as the solid blockage scenario is concerned, it is suggested to investigate numerically the effect of the specific material properties of the internal electrical heater on the heat flux distribution inside the pin cladding, since in the experimental campaign technical report no precise indication has been given, and commercially it is possible to find very different properties for the same material considered. Additionally, such model should be combined also with an electrical one, where it could be possible to investigate the impact of the presence of the blockage on the electrical resistance and current flow.

Considering the porous blockage instead, further numerical simulations will allow to make a specific and more quantitative assessment of the real impact of porosity and self-heating of the porous blockage. For example, by establishing the effective maximum cladding temperature, it will be possible to evaluate which are the conditions that will lead to the initiation of pin failure.

In conclusion, one can highlight the necessity of carrying out experiments to further investigate these aspects and to better understand the effect of location of blockages: despite the temperature shoot up in case of these active local blockages might be excessive and lead to pin failure, the presence of local active blockages is detected rapidly thanks to the delayed neutron detection signal [74]. On the other hand, local cold blockages can jeopardize more the safety of the core: their detection through changes in the reactivity in the reactor is not immediate, in addition to the fact that the pressure drop across them is limited and the overall mass flow rate is marginally affected. Hence, albeit the outlet flow conditions do not change sufficiently to allow for a prompt presence determination. Yet, in the eventual case that the occurring local hot spots lead to pin cladding failure, the fuel leakages can be detected by the fission gas release.

Ultimately, although the local blockage detection is of paramount importance in order to avoid the initiation of accidental scenarios and propagation of core damage, it is relevant to highlight that, even in the range of temperatures obtained in the analysed worst case scenario (high power generation and low mass flow rate), the criterion of core damage propagation is unlikely to be

met. In fact, according to the cladding burst criterion, cladding failure in a short-term transient is expected above $\approx 930^{\circ}\text{C}$. It is true that creep effects start to have an impact on the long term above $\approx 550^{\circ}\text{C}$ and that higher the temperature, the faster the occurrence of failure; nevertheless, even if local blockages are not immediately detected, the creep effect would not be important yet.

In the end, it is important to keep in mind that the aim of the present work is the validation of the numerical CFD method against experimental data. Therefore, given the introduction of innovative features, like for instance the liquid metal coolant, there is the need to assess the safety of the installation by studying the performance of the primary cooling system, also in accidental conditions, via performing several representative experiments. Indeed, the modelling of liquid metals flows in channels with particular geometries as the one of interest is still not a well mastered field, given all the related peculiar features and complexities, thus necessitating of a more detailed study using mock-ups of the real physical geometry.

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Appendix A – Detailed description of the background experimental campaign and numerical simulation

A.1 Experimental background context

Within the European Project MAXSIMA, internal flow blockages scenarios in fuel rod cluster have been investigated, given their likelihood of producing rather important local hot spots that could eventually lead to cladding failure. Here below it is possible to acknowledge the specific information regarding the thermal-hydraulic effects of such elements in the 19-pin LBE-cooled and electrically heated rod bundle present in the THEADES loop at KIT-KALLA, under operating conditions representative of the ones expected for the MYRRHA reactor and conservative blockage scenarios characteristics approach.

A.1.1 Test section

The experiments have all been performed in the already instrumented loop visible in Figure 74, where liquid LBE is flowing (see the detailed information of the test facility in [50], [58]).

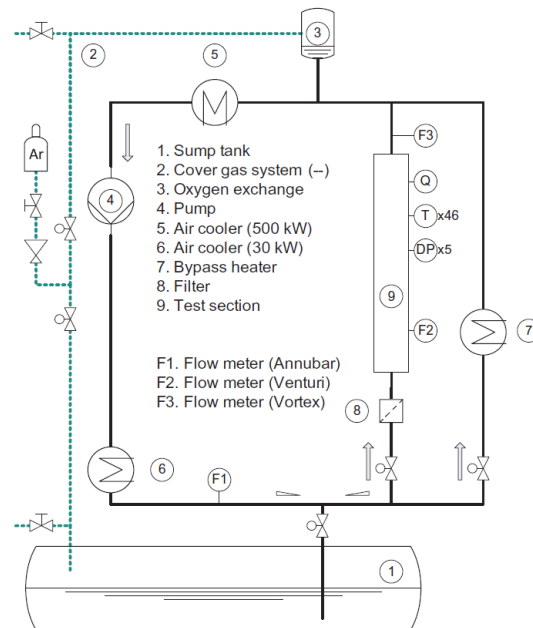


Figure 74 – Sketch of the THEADES loop installation [50]

The test section, as already showed in Figure 7, is a bundle of 19 electrically-heated rods with internal blockages embedded in an hexagonal channel, all inserted into an outer pressure vessel. In Table 15 below are listed the specific dimensions of the test section present in the THEADES loop at KIT-KALLA.

Dimension	Symbol	Value	Unit
<i>Heated rods</i>			
Rod outer diameter	D	8.2	mm
Rod total length	L_{tot}	2229	mm
Rod heated length	L_{heat}	870	mm
<i>Triangular array of 19 rods</i>			
Pitch	P	10.49	mm
Ratio	P/D	1.279	–
Wall distance	W	10.58	mm
<i>Wire spacers</i>			
Wire diameter	d	2.2	mm
Wire axial pitch	H	328	mm
Ratio	H/D	40	–
<i>Hexagonal flow channel</i>			
Apothem	a	24.65	mm
Corner curvature	r	2.5	mm
Flow area	A_{hdl}	1027.26	mm ²
Wet perimeter	P_{hdl}	789.95	mm
Hydraulic diameter	$d_{h,hdl}$	5.2016	mm
<i>Internal sub-channel</i>			
Flow area	A_{sch}	19.34	mm ²
Wet perimeter	P_{sch}	16.34	mm
Hydraulic diameter	$d_{h,sch}$	4.7362	mm

**Main geometrical parameters of the test section
at THEADES loop at KIT-KALLA**

Table 15 – Principal geometrical parameters of the reference test section at THEADES loop at KIT-KALLA [58]

It is extensively instrumented with several sensor devices and probes, which serve for the measurement of flow rate (volumetric flow meters, Vortex flow meter, Venturi nozzle), differential pressure, temperature (thermocouples) and power, all adequately calibrated. In specific, the latter is provided by direct-current supply, in order to heat all the rods simultaneously, and measured by independent voltage and current measurements. Therefore, the electrical power obtained leads to a uniform heat flux in all the pins since the heaters have the same electrical resistance.

Furthermore, it is important to mention that all the transient recorded data within the campaign tests are time-averaged, in order to obtain a steady state analysis.

A.1.2 Blockage material properties

As mentioned before, solid blockages represent the worst-case accidental scenario, therefore the chosen material should be solid and characterised by a low thermal conductivity, so to exemplify the safety concerns of LBE cooled systems. Indeed, in the experiments the reference case analysed considers lead oxide (PbO), that has a thermal conductivity between 1.0 and 1.5 W/(mK) at 500°C and 90% theoretical density. Other stringent requirements are the chemical and physical stability in high temperature LBE environment and practical machinability, as well as a thermal expansion coefficient similar to the one of steel, in order not to damage the surrounding rods.

For this reason, so that all the requirements are met, it has been chosen to fabricate a heterogeneous blockage with a pourable ceramic material based on silicon oxide, encased in a thin-walled stainless-steel shell. The temperature dependant properties of these materials are listed in Table 16 for the stainless steel shell and in Table 17 for the ceramic filling material.

$T, ^\circ\text{C}$	$\lambda(T), \text{W m}^{-1} \text{K}^{-1}$	$c_p(T), \text{J kg}^{-1} \text{K}^{-1}$	$\rho(T), \text{kg m}^{-3}$
20	13.20	493.31	7864.5
100	15.24	500.10	7825.1
200	16.95	508.73	7782.8
300	18.32	517.50	7744.1
400	19.65	526.43	7703.9
500	21.01	535.51	7653.2
600	22.40	544.74	7606.5
700	23.84	554.14	7558.3
800	25.34	563.69	7508.4
900	26.92	573.42	7457.0
1000	28.57	583.31	7403.8
1100	30.30	593.37	7349.0
1200	32.13	603.60	7292.4

Table 16 – Temperature dependant thermophysical properties for the steel shell [59]

$T, ^\circ\text{C}$	$\lambda(T), \text{W m}^{-1} \text{K}^{-1}$	$c_p(T), \text{J kg}^{-1} \text{K}^{-1}$	$\rho(T), \text{kg m}^{-3}$
27	1.500	600	2071
100	1.366	711	2071
200	1.244	843	2071
300	1.084	897	2071
400	1.009	960	2071
500	0.951	1017	2071
600	0.972	1052	2071

Table 17 – Temperature dependant thermophysical properties for the blockage paste [75]

A.2 Numerical background context

Within the European Project MAXSIMA, internal flow blockages scenarios in fuel rod cluster have being investigated, given their likelihood of producing rather important local hot spots that could eventually lead to cladding failure. Here below it is possible to acknowledge the specific information regarding the numerical CFD simulations performed by NRG as support to the safety analysis for the MYRRHA reactor on the influence of such elements on the LBE flow in a 19-pin wire-wrapped rod bundle.

A.2.1 Computational setup

As visible in Figure 75, the computational domain is based on the geometry of the 19-pin wire-wrapped fuel bundle described already in the paragraph “A.1.1 Test section”, except for the wire that has been modelled differently compared to the design shape of the test facility, in order to avoid meshing the contact point between the rod and the wire. [75]

As already mentioned in the description above, the modelled domain length is long enough to allow for flow development, and the internal electrical setup hasn't been included, meaning that the power is applied uniformly on the inside surface of the steel cladding.

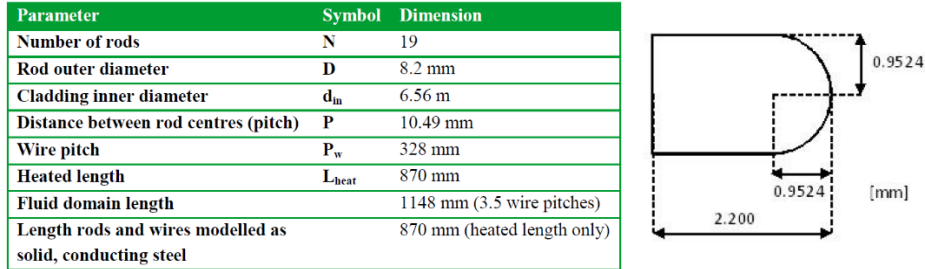


Figure 75 – Geometrical dimensions of the computational domain (left), sketch of the wire shape adopted (right) [46]

A.2.2 Blockage properties specification

Based on the experimental setup and technical specifications of the test section, the properties of the blockages refer to the ones of the materials practically used for the tests (see “A.1.2 Blockage material properties”). In Table 18 the specific expressions implemented in the CFD code are listed.

	Stainless steel shell DIN 1.4571	Ceramic paste	
Density [kg/m ³]	$\rho(T) = 8040.3 - 0.44165 * T + 2.071 * 10^{-5} * T^2 - 5.8048 * 10^{-8} * T^3$	8000	
Specific heat [J/kg K]	$c_p(T) = 456.2817 + 0.4337 * T - 5.7714 * 10^{-4} * T^2 + 3.5074 * 10^{-7} * T^3$	502	
Thermal conductivity [W/m K]	$\lambda(T) = 13.28571 + 1.756205 * 10^{-2} * T - 5.378788 * 10^{-6} * T^2 + 4.292929 * 10^{-9} * T^3$	27	1.5
		100	1.366
		200	1.244
		300	1.084
		400	1.009
		500	0.951
		600	0.972

Table 18 – Temperature dependant thermophysical properties for the steel shell [77] and blockage paste [45] (T in [°C])

Appendix B – Numerical modelling theory

B.1 Turbulence modelling

Turbulent flows are characterised that fluctuating velocity fields, as well as the transported quantities, like momentum and energy. For the turbulent flow computation, a procedure based on Reynolds-averaged Navier Stokes (RANS) equations is carried out. These equations, expressed in Equations 7 in Cartesian coordinates, are obtained from the time-averaging of the Navier-Stokes and continuity equations for an incompressible flow (Equations 5).

$$\begin{cases} \text{div } \mathbf{u} = 0 \\ \frac{\partial \mathbf{u}}{\partial t} + \text{div}(\mathbf{u}\mathbf{u}) = -\frac{1}{\rho} \frac{\partial p}{\partial \mathbf{x}} + \nu \text{div}(\text{grad}(\mathbf{u})) \\ \frac{\partial \mathbf{v}}{\partial t} + \text{div}(\mathbf{v}\mathbf{u}) = -\frac{1}{\rho} \frac{\partial p}{\partial \mathbf{y}} + \nu \text{div}(\text{grad}(\mathbf{v})) \\ \frac{\partial \mathbf{w}}{\partial t} + \text{div}(\mathbf{w}\mathbf{u}) = -\frac{1}{\rho} \frac{\partial p}{\partial \mathbf{z}} + \nu \text{div}(\text{grad}(\mathbf{w})) \end{cases} \quad (5)$$

Specifically, the instantaneous governing Navier-Stokes equations have to be averaged to remove the small time scales present in turbulent flows at realistic Reynolds numbers, because generally smaller than the smallest finite volume mesh that could be used in numerical analysis [78]. This time average is possible when considering scales much larger than the ones of the turbulent fluctuations, but yet smaller than the time scale at which the equations are solved. The instantaneous quantities, like the velocity, can then be represented by time-averaged and a fluctuating component respectively: $\vec{v} = \bar{\vec{v}} + \vec{v}'$, where the average component is:

$$\bar{\vec{v}} = \frac{1}{\Delta t} \int_t^{t+\Delta t} \vec{v} dt \quad (6)$$

Therefore, after substituting the average quantities into the above-mentioned set of transport equations, the following are obtained, where the continuity equation does not change [79]:

$$\begin{cases} \text{div } \mathbf{U} = 0 \\ \frac{\partial \mathbf{U}}{\partial t} + \text{div}(\mathbf{U}\mathbf{U}) = -\frac{1}{\rho} \frac{\partial P}{\partial \mathbf{x}} + \nu \text{div}(\text{grad}(\mathbf{U})) + \frac{1}{\rho} \left[\frac{\partial(-\rho \overline{u'^2})}{\partial x} + \frac{\partial(-\rho \overline{u'v'})}{\partial y} + \frac{\partial(-\rho \overline{u'w'})}{\partial z} \right] \\ \frac{\partial \mathbf{V}}{\partial t} + \text{div}(\mathbf{V}\mathbf{U}) = -\frac{1}{\rho} \frac{\partial P}{\partial \mathbf{y}} + \nu \text{div}(\text{grad}(\mathbf{V})) + \frac{1}{\rho} \left[\frac{\partial(-\rho \overline{u'v'})}{\partial x} + \frac{\partial(-\rho \overline{v'^2})}{\partial y} + \frac{\partial(-\rho \overline{v'w'})}{\partial z} \right] \\ \frac{\partial \mathbf{W}}{\partial t} + \text{div}(\mathbf{W}\mathbf{U}) = -\frac{1}{\rho} \frac{\partial P}{\partial \mathbf{z}} + \nu \text{div}(\text{grad}(\mathbf{W})) + \frac{1}{\rho} \left[\frac{\partial(-\rho \overline{u'w'})}{\partial x} + \frac{\partial(-\rho \overline{v'w'})}{\partial y} + \frac{\partial(-\rho \overline{w'^2})}{\partial z} \right] \end{cases} \quad (7)$$

The extra stress terms, known as Reynolds stresses, have been clearly expressed and they are the consequence of the non-linear convective term in the un-averaged equations. They represent the enhanced transport processes above the level possible by molecular effects caused by the turbulent velocity fluctuations, because these latter occur at a much larger length scale compared to the

mean free path of the molecular fluctuations, leading to the predominance of the turbulent fluxes with respect to the molecular. [80]

Though, in addition to the RANS equations, which are able to give information on the time-averaged properties of the flow, turbulence models are needed in order to have a description of the effects of turbulence on the mean flow, because they are able to predict the Reynolds stresses and the transport of the scalar terms. The classification of the RANS turbulence models is based on the number of additional transport equations that have to be solved together with the RANS flow equations. The most used and validated models are the “Mixing length model” (0 equations), the “Spalart-Allmaras model” (1 equation), the “ $k-\varepsilon$ model” (2 equations) and the “ $k-\omega$ model” (2 equations) belonging to the so called Eddy viscosity models, and the Reynolds stress models.

Although the easiness of implementation of the 0-equation model and its very fast computation time, it is not adequate for complex turbulence problems, since it is incapable to describe flow with separation and recirculation. The Spalart-Allmaras model is not suitable either, due to the non-sensitivity to the transport process in rapidly changing flow conditions and it is not accurate for internal flows. For these reasons, the description of the others aforementioned class of models will be given below, being also the ones used in the simulations developed in this thesis.

Eddy viscosity models rely on the Boussinesq approximation, which postulates the relation among the Reynolds stresses, the mean velocity gradients and the eddy viscosity through the gradient diffusion hypothesis. These models are nevertheless limited in the modelling of three-dimensional and anisotropic flows or flows presenting sudden changes in mean strain rate, because the eddy viscosity is a property of the type of flow, rather than of the fluid itself, and therefore there is not clear correlation between the Reynolds stresses and the velocity gradient. [81]

Opposingly, the Reynolds stress models (RMS) don't rely on the Boussinesq approximation, so no relation is assumed and thus they solve one additional equation for each unknown of the Reynolds stress tensor. Since every component is modelled, these models are suited for the modelling of anisotropic flows and the solution is in principle more accurate. Nonetheless, it is computationally expensive due to the big increase in the number of additional equations to be solved and the presence of terms that have still to be modelled. [60]

B.1.1 $k-\varepsilon$ model

This turbulence model requires two additional PDEs to be solved, namely one for the turbulent kinetic energy per unit mass k and the other for the turbulent dissipation rate ε , and it focuses on

the mechanisms affecting the turbulent kinetic energy. Among the advantages: the relatively easy implementation, because of the need of the supply of only boundary conditions, and the quite fast convergence, leading consequently to a computationally cheap model, widely used for the prediction of many flows. On the other hand, this model is not able to predict accurately rotating flows or with strong separation, where the biggest drawback is the lack of sensitivity for adverse pressure gradients. Furthermore, it is not able to solve flows driven by anisotropy of normal Reynolds stresses, e.g. fully developed flows in non-circular ducts.

Given the well-known shortcomings of the $k-\varepsilon$ model, some modifications have been made to develop other two equations models based on it, such as:

- *$k-\varepsilon$ RNG model*: it derives the additional two equations from a rigorous statistical technique called “Renormalization Group Method”. Similar to the standard $k-\varepsilon$, it includes improved predictions for high streamline curvature and strain rate, transitional flows and wall heat and mass transfer. It is still not suitable for the spreading of a round jet;
- *Realizable $k-\varepsilon$ model*: it contains the same turbulent kinetic energy equation of the standard model, whereas the equation for ε is improved. It has demonstrated enhanced performance for flows involving planar and round jets, strong streamline curvature and recirculation.

B.1.2 $k-\omega$ model

In this case, the additional two PDEs needed are a modified version of the turbulent kinetic energy per unit mass k compared to the previous models and one for the turbulence frequency ω , that is the inverse time scale associated with the turbulence. The power of this model is its exceptional performance for wall bounded and low Reynolds number flows, working significantly better in case of adverse pressure gradients conditions. Oppositely to the $k-\varepsilon$ model, it does not require damping functions and has straightforward Dirichlet boundary conditions allows for a significant numerical stability. Yet, it under predicts the amount of separation for severe pressure gradients flows.

As it occurred already above, some variations of the standard model have been developed to improve its performances, like the *SST $k-\omega$ model*. The Shear Stress Transport (SST) model is a combination of the $k-\varepsilon$ model in the fully turbulent region and the $k-\omega$ model in the near wall region, exploiting a blending function based on wall distance in order to calculate the turbulence variables such as dissipation, production and stress tensor. The expression for the eddy viscosity

is modified in such a way that it accounts for the transport effect of the principal turbulent shear stress. The advantages obtained are the increased accuracy in the prediction of flow separation under adverse pressure gradients, therefore it is recommended for high accuracy boundary layer simulations. Nevertheless, it requires fine mesh resolution near the wall, therefore it is computationally heavy and expensive.

B.1.3 BSL Reynolds Stress model

As mentioned before, this turbulence model involves an additional independent equation for each component of the Reynolds stress tensor. Similarly as before, it occurs that the solution is both ϵ and ω based, being this model able to switch between the formulations depending on the distance from the wall to reach a low Reynolds number formulation near the wall. [60]

B.2 Wall treatment

Since the modelling of the region close to the wall affects significantly the accuracy of the numerical results, it is relevant to have a better understanding of the representation of the flow characteristics in the so-called boundary layer region. The boundary layer is the fluid region close to a bounding surface where viscosity plays a significant role [80]. As represented in Figure 76, the velocity profile of a steady flow develops when it comes into contact with the flat plate: the boundary layers starts at the stagnation point at the edge of the plate, then it develops with a laminar behaviour. When the boundary layer reaches a certain thickness, the viscous interaction between the flow and the boundary is not sufficient to keep the laminar regime. The transition to the turbulent regime is caused therefore by disturbances within the flow, namely shear forces created at the interface between adjacent particles, and when the a time-variable velocity (in direction as well as magnitude) at any position is reached, the flow is considered fully turbulent. Here, the region closest to the boundary (viscous sublayer) is governed by the viscous forces, where the velocity profile is laminar, due to the no-slip condition at the wall. Further in the bulk, the flow is turbulent (“turbulent core”) and the velocity profile presents fluctuations and eddies establish. These eddies significantly increase the momentum and energy transfer rate across the mean flow direction.

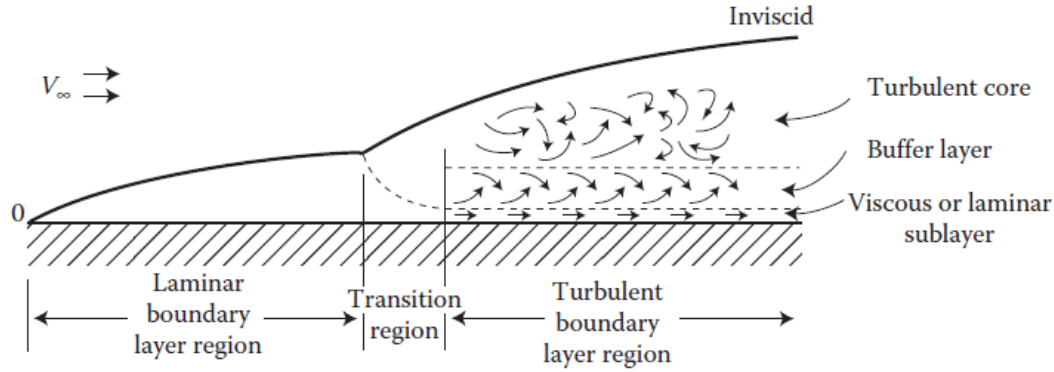


Figure 76 – Boundary layer velocity distribution for flow on an external surface [80]

It is clear from this example then, that the presence of walls greatly affects turbulent flows, since the mean velocity flow has to satisfy the no-slip condition at the wall and the viscous forces reduce the tangential velocity fluctuations. On the other side, the bulk of the flow behaves differently, due to the big gradients in the mean velocity that lead to turbulence enhancement from the production of turbulence kinetic energy. In conclusion, the big change in variables occurring in the boundary layer constitutes an issue for the accurate representation and resolution of the region.

In numerical modelling, the boundary layer regions are usually differentiated by the dimensionless parameter y^+ . This parameter represents the adimensional wall distance for a wall-bounded flow and it is defined as $y^+ = \frac{y u^*}{\nu}$, where $u^* = \sqrt{\frac{\tau_w}{\rho}}$ is the friction velocity, ν is the kinematic viscosity and y is the distance of the first cell centroid from the wall. Therefore, for values of $y^+ < 5$ the viscous sub-layer is identified, since at the wall the fluid is stationary and dominated by viscous effects. Outside this region, for values $30 < y^+ < 500$, the logarithmic-law layer can be found, where viscous and turbulent effects are more important. In between ($5 < y^+ < 11$) there is the buffer layer, which is characterised by the maximum turbulence production. [79]

As anticipated before, depending on the value of this parameter, the turbulence models treat differently the near wall region. Low-Reynolds number models use refined mesh at the wall, i.e. $y^+ \sim 1$, in order to resolve the key phenomena also in the viscous sub-layer, where the wall shear stress is computed as in laminar flow. Thus, albeit the better modelling of the viscous sublayer is achieved, the computational cost is greatly increased.

On the other hand, high Reynolds number models use wall functions, which are equations empirically derived and used to satisfy the physics in the near wall region. In this latter family of models, the first cell centroid needs to be located in the fully turbulent region, and consequently

the viscous sublayer resolution is not significantly accurate, however it allows to save a considerable number of cells near the wall. Additionally, the other big concern is related to the location of the first cell centroid, being the predictions very sensitive to it: in case of a too refined mesh, only a partial resolution of the boundary layer will be obtained. In CFX this issue is tackled by the implementation of scalable wall functions: the model automatically moves the first node at the intersection between the viscous sublayer and the logarithmic-law region, when it is originally placed in the viscous sublayer, allowing to apply it to fine meshes and perform mesh refinements independently on the Re number. [60]