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## DEVELOPMENTS IN SINGLE PHASE FUEL ASSEMBLY SIMULATIONS

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#### **Abstract**

The heart of every nuclear reactor is the core where the nuclear chain reaction takes place. Heat is produced in the nuclear fuel and transported to a coolant. Most core designs consist of many fuel assemblies which in turn consist of a large number of fuel rods. In most fourth generation reactor concepts (and also in pressurized water reactors), single phase heat transfer plays an important role. For the design and safety analyses of such reactors, simulations of the heat transport within the core are essential. This paper will demonstrate the single phase CFD validation approaches that have been performed by the authors focusing mainly on liquid metal and supercritical water coolants. For turbulence modeling, RANS, URANS, and LES approaches have been applied. It will be demonstrated that CFD analyses indeed support the development of improved heat transfer correlations for application in system codes.

### Introduction

The nuclear chain reaction, which is the source of nuclear fission energy production, takes place in the core of a nuclear reactor. Within this core, heat is produced in nuclear fuel and transported to a coolant. Mostly, nuclear cores consist of a few hundred fuel assemblies which in turn consist of a large number of fuel rods. In pressurized water reactors, but especially also in most fourth generation reactor concepts, single phase heat transfer plays therefore an important role in the thermal-hydraulic evaluation of the reactor core. For the design and safety analyses of such reactors, simulations are required at system level using system codes like e.g. RELAP. In these system codes, the heat transport within the core is essential and is taken into account by means of correlations. However, the heat transfer correlations for liquid metal and supercritical water coolants contain large uncertainties. Experiments and CFD simulations play an important role to close this knowledge gap. As experimental data is often hard to obtain and very costly, nuclear reactor designers rely more and more on simulation techniques like CFD.

This paper will demonstrate the single phase CFD validation approaches that have been performed by the authors focusing mainly on liquid metal and supercritical water coolants. The paper first discusses the validation work on bare rod bundles in section 1. A specific issue when discussing the flow in bare rod bundles deals with flow pulsations like elaborately discussed by [1]. As already mentioned, CFD is foreseen to play a significant role in the derivation and optimization of existing heat transfer correlations like e.g. reported by [2, 3, 4, 5]. The work of the authors on rod bundles with grid spacers and wire wraps are presented in section 2 and section 3, respectively. Simulation of rod bundles with grid spacers and wire wraps are presented in section 3. Although limited validation is available in open literature concerning grid spacers, more information is available about wire wraps. Apart from that, [6,

7, 8] have reported CFD simulations based on RANS and LES techniques for wire wrapped rod bundles. Section 4 and section 5 will present applications to inter-fuel assembly flow and effects of partial or complete blockages.

#### 1. Bare Rod Bundles

In order to simulate the heat transport in the core of a nuclear reactor, a correct description of the flow behaviour of bare rod bundles, i.e. rod bundles without any grid spacers or wire wraps guiding the flow, is a first prerequisite. In bare rod bundles, the flow patterns are governed by the interaction of the fluid flow with the rod walls. Therefore, prediction of the fluid behaviour near the walls is very important. With the introduction of grid spacers or wire wraps, the complexity of the simulations, normally shifts to the geometric modeling although near wall behaviour remains important.

## 1.1 Step-wise Validation

For the design and safety analyses of nuclear reactors, simulations of the heat transport within the core are essential. However, for innovative reactors, the specific correlations for heat transport often contain large uncertainties. Therefore, experiments and CFD simulations play an important role in order to close this knowledge gap. As experimental data for coolants used in innovative reactors is often hard to obtain and very costly, nuclear reactor designers rely more and more on simulation techniques like CFD. However, CFD approaches first need to be validated against experimental data.

A numerical engineering modeling approach using CFD with Reynolds Average Navier Stokes (RANS) turbulence modeling was developed and validated for liquid metal coolants using a stepwise approach described in more detail in [9]. As a first step, CFD simulations were conducted for the heat transport in liquid metals in straight tubes. Results were compared to empirical correlations. In the second step, CFD simulation results were compared to single heated rod experiments performed at KIT in Karlsruhe. The third step was to compare the hydraulics in a rod bundle to experimental results obtained in simulation fluids like e.g. water or air. Such fluids allow relatively easy, less costly and often more accurate measurements than liquid metals as shown e.g. by Schulenberg and Stieglitz [10]. The last step is to compare thermal-hydraulic simulation results to experimental results obtained in a liquid metal rod bundle geometry. To this purpose, the four rod sodium TEGENA experiments in Karlsruhe [11] were used. This stepwise development and validation campaign has lead to clear recommendations and conclusions for a RANS-based CFD approach summarised in [10].

For supercritical fluids, a similar stepwise validation procedure is followed. First, simulations are performed for supercritical fluid flow in straight tubes. Relevant experimental data is available for such cases to which numerical simulations can be compared. The well known data from Yamagata [12] was used in [13] to get a first impression of the feasibility of current RANS turbulence models to simulate supercritical fluids. After that [14] used the data of Herkenrath [15] for simulation at more relevant mass and heat fluxes. This was followed by [16] which compared to new experimental results obtained by Kim et al. [17]. Recently, also comparisons have been made to experimental data from Mori et al. [18]. All these validation steps indicate that the SST k-ω seems a suitable candidate to predict the heat transfer of supercritical fluids qualitatively. However, quantitatively large improvements are required. In a second step, simulation results are compared to single heated rod experiments in an annulus. Such data is available from [19] and is assessed by [20]. Furthermore, new data will become available in 2011/2012 from the experimental DeLight facility under construction at the university of Delft as part of the European FP7 THINS project [21]. The third step is to compare numerical simulations with

actual rod bundle data. Experimental results are obtained by [22] in their experimental supercritical Freon 7 pin rod bundle. Figure 1 shows preliminary numerical results which were obtained from simulating a 30° section of this 7 pin supercritical Freon rod bundle. Based on previous experience (see e.g. [20]) the SST k-ω turbulence model was selected for the simulations. The graph in figure 1 shows the evolution of temperature profiles along with the computed bulk enthalpy. The average wall temperature is indicated by Tw\_avg. In addition, the axial temperature distribution along the north and east wall is shown. This demonstrates the deviations from the average. A good agreement is shown for the average temperature with the experimental data indicated in the same graph.

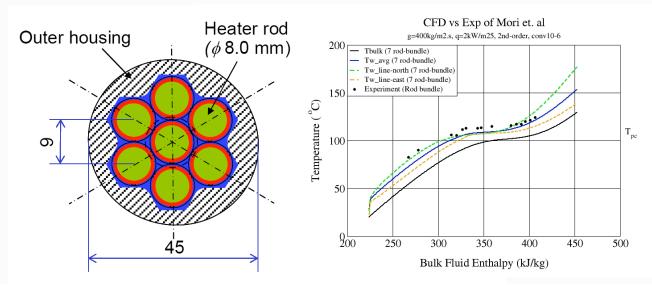


Figure 1 Preliminary results for simulation of a 7 pin bare rod bundle with supercritical fluid.

## 1.2 Flow Pulsations

The history of the discovery of flow pulsations in rod bundles is extensively discussed in [1]. The hydraulics experiments by Hooper and Rehme [23] and the thermal-hydraulics experiment by Kraus and Meyer [24] revealed the existence of such flow pulsations in a tightly spaced rod-bundle with pitch-to-diameter ratio (p/d) of 1.1 and 1.06, respectively. These flow oscillations can cause flow-induced vibration in a rod-bundle, see e.g. [25], [26], and [27]. It has been revealed by the thermal-hydraulics experiment that these flow oscillations result in temperature oscillations [24]. These temperature oscillations in turn can induce thermal shock or thermal fatigue damage to the walls of the rods in a bundle as e.g. analyzed extensively for mixing flows in T-junctions, see e.g. [28], [29], and [30]. To capture such time-dependent flow features an Unsteady RANS, a Large Eddy Simulation (LES), or even a Direct Numerical Simulation (DNS) approach is needed, see e.g. [31] and [32]. An assessment was made of URANS and LES modeling approaches by analyzing Hooper's hydraulics experiment [23]. A three dimensional perspective of URANS and LES analyzed axial velocity is shown in figure 2. This figure shows:

- A wavy pattern that can be inferred from the regions with different axial velocities in the analyzed mid-plane. These are indicated by arrows in the figure. As expected, the velocity is lower in the smallest gap region and higher in a region close to the open boundaries.
- The presence of smaller flow structures in the LES computed flow field in comparison to URANS computed flow field. For instance, small plumes of low velocity are observed at the inlet section in LES and are not visible with URANS computation.

The presence of smaller flow structures in LES is attributed to smaller values of analyzed turbulent eddy viscosity in comparison to URANS. In general, analyzed effective viscosity with LES is lower than that of URANS with the generated grid and employed computational frame-work.

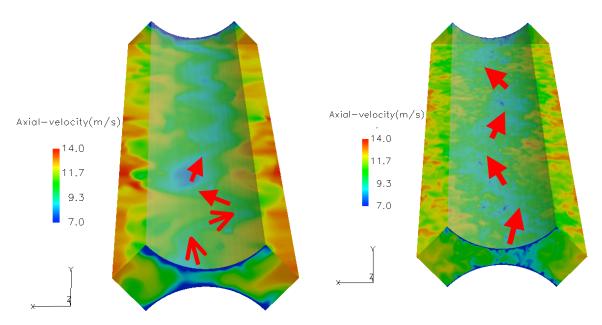


Figure 2: URANS (left) and LES (right) analyzed axial velocity after about 1s of computational time.

Power Spectral Densities (PSD) of the URANS and LES analyzed axial velocity fluctuations at two different measurement points are shown in figure 3. The analyzed axial velocity fluctuations over six and eight flow-through times are employed for this purpose in the adopted URANS and LES approaches, respectively.

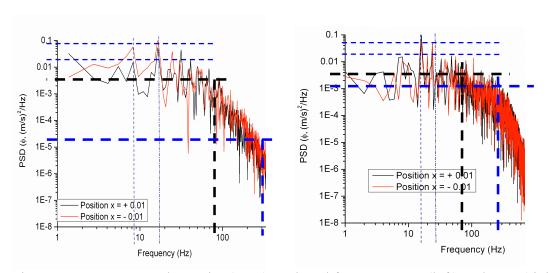


Figure 3 Power Spectral Density (PSD) analyzed from URANS (left) and LES (right) analyzed axial velocity fluctuations.

The velocity fluctuations indicate:

- The PSD peaks are observed in the production frequency range of 10-20 Hz for URANS and in the range of 17-27 Hz for LES analyzed axial velocity fluctuations. These frequencies are associated with the dominant amplitudes (e.g.  $\pm$  1.5 m/s) of axial velocity fluctuations.
- [23] indicates that the average characteristic frequency of the observed large scale structures is about 30 Hz. The LES analyzed results show a closer resemblance with the experimental observation than that of URANS analyzed results. This indicates the presence of large scale structures that contribute to a higher production of turbulence energy or power in the indicated frequency ranges.
- It can be observed that the energy of turbulent structures with a frequency of about 300 Hz is much smaller in URANS in comparison to LES. This can be attributed to a higher eddy-viscosity in the URANS approach compared to LES. This means, smaller scales with such a high frequency in URANS are not sustainable whereas they still exist in LES. At the same time, energy contents of turbulent structures with frequency below 100 Hz are comparable in URANS and LES. In other words, URANS will be useful for applications where lower frequencies or larger or mean flow structures are relevant.

More details of the described analyses can be found in [33]. The LES simulations presented in this framework should be considered as preliminary. LES simulations with finer grids are underway at NRG for Hooper's experiment and other experiments showing flow pulsations.

## 1.3 Derivation of Heat Transfer Correlations

Many heat transfer correlations are available in literature for liquid metals which show a wide spread of results. In order to select an appropriate correlation for the simulation of the European Lead cooled System (ELSY) [34], CFD analyses were performed and results were compared to existing correlations described by Mikityuk [3]. From the existing correlations, the correlations of Ushakov and Gräber were selected for triangular arrangements, the correlation of Zhukov was selected for square arrangements and Mikityuk's general empirical correlation was selected which should be suitable for both arrangements. All these correlations were derived for a certain pitch-todiameter range. However, the purpose of this study was to select a correlation independent of the exact pitch to diameter ratio, is this was not fixed yet in the pre-conceptual design of ELSY. The CFD based Nusselt number has been obtained by using  $Nu = q_w \cdot D_h/k \cdot (T_{max} - T_{mean})$ , with  $q_w = wall$ heat flux,  $D_h$  = hydraulic diameter,  $T_{mean}$  = surface averaged lead temperature,  $T_{max}$  = maximum wall temperature and k=thermal conductivity. It should be emphasized that the maximum wall temperature has been employed for computing these Nusselt numbers. These computed conservative Nusselt numbers have been averaged over several axial positions near the assembly outlet to obtain average Nusselt numbers. This method can be considered reasonable as the Nusselt numbers remains almost the same in a fully developed flow and temperature regime. A comparison between CFD computed and correlations based Nusselt numbers is provided in [9]. They show that the average Nusselt number increases with pitch-to-diameter ratio for both arrangements, which is consistent with the findings reported in [35]. For a square arrangement of a bare and liquid metal cooled rod-bundle, the CFD computed average conservative Nusselt numbers give the best agreement with Zhukov's correlation in the considered range of pitch-to-diameter ratio. Whereas in case of a triangular arrangement of bare and liquid metal cooled rod-bundle, deviations between RANS analyzed average Nusselt number values and Mikityuk's correlation are the least. Consequently, in the investigated range of pitch-to-diameter ratio, Mikityuk's correlation is preferred over other correlations for a triangular arrangement of rod-bundle.

With the aim of deriving a heat transfer correlation suitable for the HPLWR design [36] including a wire wrap as a spacer, an extensive set of RANS CFD analyses was performed in cooperation with the universities of Stuttgart in Germany and Stockholm in Sweden [37]. A single heated pin both in an annulus and in a square channel, a single centre sub channel and a small assembly of 4 heated pins have been studied. All geometries have been modeled separately with and without the presence of a wire wrap. RANS CFD results have been used to derive correction factors to update a base correlation from literature to account for the effect of the wire-wrap and the effect of the geometry of the HPLWR fuel assembly.

The correlation by [4] valid for super-critical water in a circular tube is selected as base correlation  $Nu_{base}$ . In the derived HPLWR heat transfer correlation the correction factor  $F_{geo}$  accounts for the effect of the rod bundle geometry and  $F_{wire}$  for the effect of the wire wrap spacer that is applied in the HPLWR fuel assembly. The heat transfer correlation proposed for the current design of the HPLWR fuel assembly has the following form:

$$Nu_{HPLWR} = F_{geo} \cdot F_{wire} \cdot Nu_{base}$$
 (1)

The geometry and wire factors have been calculated using RANS analyses of several representative geometries. Based on these analyses the following factors are recommended:  $F_{geo} = 0.6$  and  $F_{wire} = 1.1$ . It should be emphasized, here, that the derived heat transfer correlation will be employed in system codes to calculate average fuel rod surface temperatures. For this purpose, in first instance average flow features and related heat transfer rates suffice.

The proposed heat transfer correlation is based on RANS CFD calculations only. The correlation could not be validated due to the lack of experimental data for rod bundles under super-critical conditions and a wire-wrap as spacer. Only a limited range of enthalpy and heat fluxes, representative for the evaporator of the three pass HPLWR core design, have been considered in the CFD analyses. Thus, further CFD analyses and CFD code validation are required to extend the range of applicability of this correlation.

#### 2. Rod Bundles with Grid Spacers

In order to predict the pressure drop occurring in the lead-bismuth rod bundle including a specific spacer grid to be tested in the KALLA experimental loop [38], RANS simulations of a 19-pin rod bundle were carried out simultaneously at KIT in Germany and at NRG [39]. For the CFD analyses, 1/3rd cross section of the water rod-bundle was selected. This allows the use of periodicity in open boundaries with grid spacers. This boundary condition is expected to allow flow redirection through these open boundaries. The modeled geometry and mesh consisting of about 8.3 million computational volumes are shown in figure 4. The total length of the modeled geometry is 1110 mm with 3 spacers separated by 370 mm. The analysed pressure drop across a spacer grid was calculated to be about 30 kPa at an average velocity of almost 9 m/s. This corresponded well with the measured pressure drop of 37 kPa at an average velocity of 10 m/s. The analysed pressure drop is also shown in figure 4.

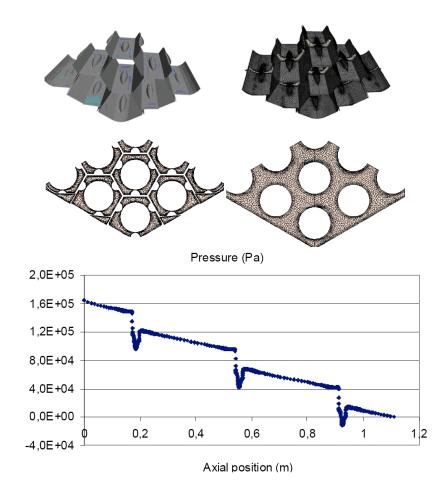


Figure 4 Spacer grid geometry and mesh and CFD based pressure drop prediction.

# 3. Rod Bundles with Wire Wraps

In a first step towards simulation of rod bundles with wire wraps, simulations [20] were performed for a supercritical CO2 tube flow with a wire wrap inserted at the inside of the tube [19]. Numerical results compared qualitatively well to the experimental results. As supercritical fluids were the object of study, it was to be expected that quantitatively there would still be room for improvement, which was already concluded for bare rod bundles (see section 1).

Numerical studies have been performed for a supercritical 4-pin rod bundle [37]. It is foreseen that similar experiments will be performed at the Shanghai Jiao Tong University in their SWAMUP facility [40] in the framework of a cooperation with the European FP7 SCWR-FQT project [41].

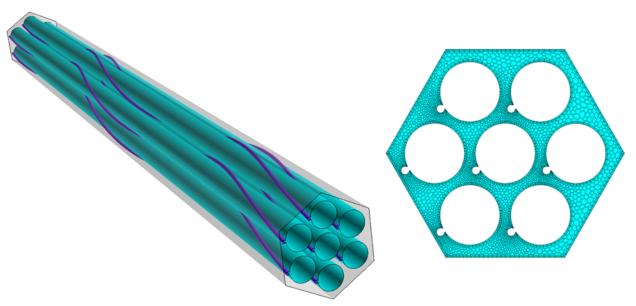


Figure 5 Geometrical set-up and employed mesh for the JAEA 7 pin rod bundle experiment

The experience in simulating rod bundles with wire wraps for supercritical fluids is currently being transferred to the simulation of a 7 pin rod bundle with wire wraps for a sodium cooled reactor. To this purpose, the 7 pin rod bundle experiment reported in [42] is being simulated with STAR-CCM+ using various RANS turbulence models in order to verify whether the often used assumption that application of advanced RANS turbulence models is not required for wire wrapped rod bundles. Figure 5 shows the geometrical set-up and the applied computational grid which exists of about 3 million computational volumes covering 2 wire pitches (mesh independency was shown using separate analyses using 4.3. million computational volumes). Apart from the standard k-ε turbulence model, also the SST-k-ω turbulence model, and the anisotropic Reynolds stress model have been employed. Intercomparison of the computational results shown in figure 6 has reveals that indeed the influence of application of advanced turbulence models is negligible. A code-to-code comparison using STAR-CCM+ and OpenFOAM has shown a good comparison between the different codes. The comparison with the experimental has revealed that the description of the experimental set-up and the results obtained in [42] is not sufficient. Further investigations are ongoing to improve the knowledge.

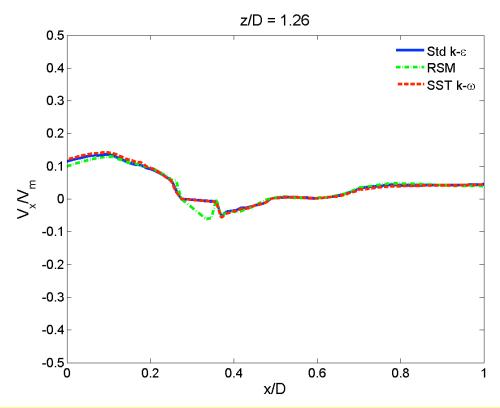


Figure 6 Comparison of local cross-velocity profiles for different turbulence models at a fixed axial position

## 4. Inter Fuel Assembly Flow in an Open Core Arrangement

Using the validated approaches described in section 2, CFD simulations are not only applied to a single subchannel of the fuel assembly of the European Lead-cooled System (ELSY) [34]. But as the reference ELSY core design existed of square open fuel assemblies, new correlations were required to describe the heat transport in the gap between two fuel assemblies as shown in figure 7.

To this purpose, the developed RANS approach was applied to a multiple subchannel domain which includes the gap between two fuel assemblies. The effect of variations of gap size were analysed, which showed that the maximum peripheral temperature difference along a rod is significant when the gap size between two fuel assemblies differs from the pitch of the rods within a fuel assembly. Such a temperature variation along a rod surface may lead to bending and ultimately in failure of the fuel rod. An optimum was found when the gap size between two fuel assemblies is chosen equal to the rod pitch within a fuel assembly. Furthermore, the heat transport between two fuel assemblies has been analysed for fuel assemblies with different power levels. For such a situation, a conservative heat transport correlation (see equation 1) has been derived which can be used in system codes. The comparison with RANS simulations for a 5.5 mm gap is presented together with more details [43].

$$Nu_{gap} \sim 10.2 - 4.7 | 1$$
-Power Ratio | (1)

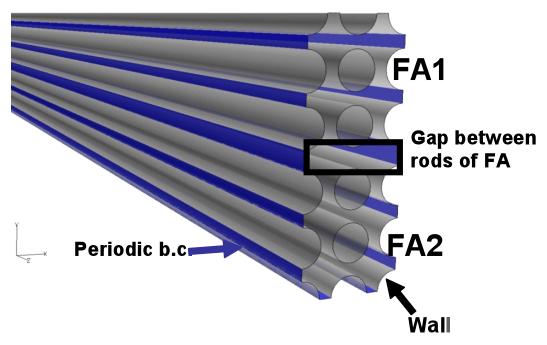


Figure 7: Fuel assemblies (FA1 and FA2) and the analysed gap region

# 5. Determination of Blockage Effects

In order to bridge the gap between traditional fuel assembly simulation approaches using system codes, subchannel codes or porous medium approaches and the detailed CFD approaches to analyze single sub-channels as described above, a Low Resolution Geometry Resolving (LRGR) CFD approach without subgrid model is described in [44]. First, a grid resolution study was performed in order to analyze the accuracy of the employed LRGR grids. Rod surface temperatures differed less than 15% to the results obtained with the detailed validated approach [9]. The LRGR CFD approach allows capturing 'medium scale' flow features such as recirculation zones, which cannot be captured by the system code, subchannel code and porous media approaches, and can serve e.g. to fine-tune the porous parameters which are important input for a porous medium approach. However, it should be noted that the prediction of detailed flow features such as secondary flows is not feasible.

Analyses using this LRGR CFD approach have shown that a partial blockage of a closed hexagonal fuel assembly design at the inlet of up to 16% cross section, leads to an average temperature increase at the assembly outlet of only ~2°C. Thus, detection of blockages at the outlet header of each single fuel assembly will strongly depend on the mixing in the outlet header. The maximum cladding temperature observed is ~673°C, so failure of fuel cladding will not occur.

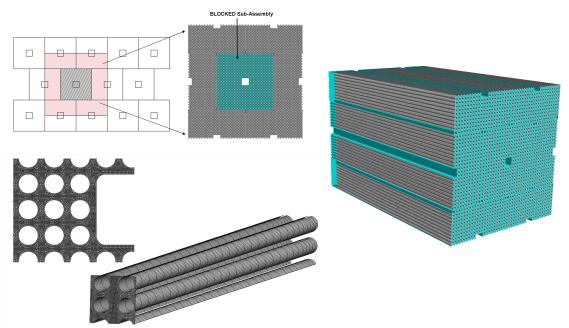


Figure 8 Computational domain and grid of the square open ELSY fuel assembly employing the LRGR CFD approach

Consequences of a large area inlet blockage of an open square fuel assembly structure were also analyzed with the LRGR CFD approach. Figure 8 shows the selected computational domain which includes an area of four fuel assemblies. This figure also reveals the employed grid for the analyses. Figure 9 shows the axial velocity and temperature contours in a vertical cross-section for a complete fuel assembly blockage. This figure reveals the large recirculation zone and the high maximum temperatures occurring behind the fuel assembly blockage. In [45] it is shown that under the assumed conditions failure of fuel cladding will occur. If there is a possibility to measure temperatures at the outlet of individual subassemblies with high precision, then an early detection of a total inlet blockage for the open square fuel assembly design might be possible. However, most probably fuel pin failure has already occurred when coolant outlet temperatures increase by a detectable amount. A time dependent simulation of consequences of an inlet blockage would become necessary to evaluate detection capabilities of massive inlet blockages by a single average coolant outlet temperature measurement at each subassembly without entering into massive fuel pin failures.

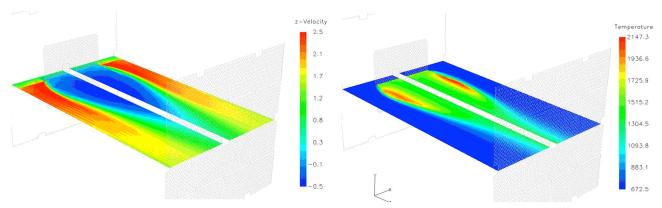


Figure 9 Axial velocity and temperature contours in a vertical cross-section for a complete open square ELSY fuel assembly blockage

## 6. Summary

This paper has demonstrated single phase CFD validation approaches that have been performed by the authors focusing mainly on liquid metal and supercritical water coolants. Firstly, simulations of bare rod bundles were discussed. Special attention was paid to validation and to the prediction of flow pulsations as observed in experiments. Furthermore, examples have been provided in which CFD played a significant role in the derivation and optimization of existing heat transfer correlations.

Simulation of rod bundles with grid spacers and wire wraps were presented. Although limited validation is available in open literature concerning grid spacers, some more information is available about wire wraps. However, for both types of spacers validation studies are underway based on comparison to experimental data available either in open literature or within the framework of a collaboration. Apart from the validation simulations performed, applications have been presented to inter-fuel assembly flow and the effects of partial or complete blockages.

Although validation of the approaches taken will always remain an important subject of the performance of any numerical simulation, it is expected that CFD will be more and more an active role in the prediction of the flow phenomena and heat transfer in nuclear fuel assemblies. Therefore, it is expected that application of the verified and validated approaches will play a larger role in future analyses.

## 7. Acknowledgements

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