

# CFD BENCHMARK FOR A HEAVY LIQUID METAL FUEL ASSEMBLY

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## ABSTRACT

As part of a Department of Energy International Nuclear Energy Research Initiative (I-NERI), the Dutch Nuclear Research and consultancy Group (NRG), the Belgian Nuclear Research Centre (SCK•CEN), Ghent University (UGent) in Belgium and the Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA) are collaborating with Argonne National Laboratory (ANL) to perform and compare a series of thermal hydraulic simulations representative of a heavy liquid metal fast reactor fuel assembly. Such a widely spaced wire-wrapped fuel assembly is a complex configuration for which few flow data are available for verification and validation of computational fluid dynamics (CFD) simulations.

For this benchmark a 19-pin wire-wrapped rod bundle with characteristics representative of the MYRRHA flexible fast research reactor, under design at SCK•CEN in Belgium, is modeled. The heat conduction in the cladding of the fuel rods and the spacer wires is taken into account by conjugate heat transfer.

UGent, ENEA and NRG performed their Reynolds Averaged Navier-Stokes (RANS) simulations with commercially available CFD codes. The high-fidelity ANL Large-Eddy Simulation (LES) was performed with Nek5000, used for CFD in the Simulation-based High-efficiency Advanced Reactor Prototyping (SHARP) suite.

The paper will show and discuss the comparison of the thermal and hydraulic RANS results and the reference Nek5000 LES results. The comparison with the LES results will indicate to which extent the current liquid metal modeling methods are sufficient and help to highlight remaining issues. The results of the study are very valuable in the design and licensing process for MYRRHA.

## 1. INTRODUCTION

The worldwide electricity demand is for about 11% supplied by nuclear power plants. Since this energy demand is rapidly growing, it suggests a persistent important role for nuclear power in the future energy supply, as outlined in the projections of the World Energy Outlook 2014 [1]. The most recent IEA/NEA nuclear technology roadmap [2] predicts in its so-called 2DS scenario a slight increase in the share of nuclear in the coming decades up to 2050, with expansion mainly occurring in Asia. The IAEA [3] attributes a large role in the future to the deployment of fast reactors. Most of the fast reactor designs [3], [4] employ either sodium or lead(-alloy) as a primary coolant. This clearly shows the importance of liquid metal coolants in the development of future nuclear energy technologies. An elaborate overview of the status of the development of fast reactors is provided in [4].

Thermal-hydraulics is endorsed as one of the key scientific subjects in the design and safety analysis of liquid metal cooled reactors. Nuclear engineers apply experiments, analytical and empirical correlations, system thermal hydraulics (STH) codes, sub-channel codes and Computational Fluid Dynamics (CFD) techniques to get an overview of the thermal-hydraulic issues and to find a solution. Due to the higher level of detail, CFD becomes more and more integrated as method for examining the thermal-hydraulics. The current status and the future challenges for CFD applied to liquid metal cooled fast reactors are summarized in [5]. A key issue for many liquid metal fast reactor thermal-hydraulic challenges is to obtain a proper validation of the CFD techniques. Therefore, liquid metal experiments and their measurement techniques should be developed simultaneously with the CFD techniques.

The work described in this paper is part of the code validation and verification approach developed in the frame of the licensing process of the Multi-purpose hYbrid Research Reactor for High-tech Applications (MYRRHA), currently under design at SCK•CEN [6]. MYRRHA is a flexible fast spectrum research reactor cooled by Lead Bismuth Eutectic. MYRRHA is identified as the European Technology Pilot Plant for the Lead Cooled Fast Reactor (LFR) which is one of the Generation IV reactor concepts [7]. As most liquid metal fast reactors, MYRRHA applies wrapped wires as spacers between the individual pins in the fuel assemblies.

A major part of CFD method validation is a code-to-code comparison on a specific thermal-hydraulic issue with different codes and different levels of modelling detail. A benchmark concerning the hydraulics in a 7-pin wire-wrapped rod bundle has been performed under the I-NERI initiative, as presented in [8]. Reference data were created from NEK5000 Large Eddy Simulations by ANL. Three Euratom members participated to this blind benchmark with Reynolds Averaged Navier-Stokes simulations: NRG using Star-CCM+, Ghent University using Fluent. The results from NRG and UGent showed good agreement with the high fidelity results from ANL. Several turbulence models were applied, showing that the cross-flow results are all equally close to Argonne's results. Further it is shown that the region in the wake of the wire is hardest to model correctly. The  $k-\omega$  SST turbulence model slightly outperforms the other turbulence models in the proximity of the wire, except for the region in the wake of the wire.

The current benchmark is an extension of the above-mentioned one. The current benchmark considers a 19-pin wire-wrapped rod bundle including conjugate heat transfer through the steel cladding and wires. Complexity is added with respect to the 7-pin benchmark at three points.

1. Geometry: the fillet radius of the wires touching the fuel rods has been reduced, leading to a more realistic geometric model but also a more challenging meshing procedure.
2. Physics: conjugate heat transfer within the cladding and the wires is applied.

3. Boundary conditions: the domain is periodic for the flow and the temperature. The periodicity for the temperature appears to be not straightforward in all codes.

Also, a fourth Euratom member joined the consortium: ENEA.

This article summarizes the computational tools and the computational setup of all partners in section 2. Also in section 2, the benchmark geometry and the benchmark exercise are described, in order to present the results in section 3 and finally the conclusions in section 4.

## **2. BENCHMARK EXERCISE**

The current benchmark consists of a 19-pin wire-wrapped rod bundle, with dimensions representative for a MYRRHA LBE-cooled fuel assembly, and corresponding to the experimental NACIE\_UP rod-bundle mock-up at ENEA. The experimental campaign is part of the European framework program 7 SEARCH project [10]. Together with the experimental campaign in the German THEADES loop at the KALLA laboratory in Karlsruhe [11], the experiments provide insight in the complexities of working with LBE as a coolant in a wire-wrapped rod bundle, relevant for the design phase of MYRRHA. Reference temperature data are produced by thermocouples at several measurement sections in the rod bundles to establish heat transfer correlations and for validation purposes. However, there is currently no realistically feasible method to produce measurements of the velocity field of the opaque LBE. Therefore this code-to-code benchmark is performed in order to validate the thermal-hydraulic results produced by pragmatic RANS simulations at UGent, ENEA and NRG with ANL's reference LES data. The temperature and conjugate heat transfer in the cladding of the rods and in the wires are included in the model, contrary to the first isothermal 7-pin benchmark. The thermal results might be compared to the NACIE\_UP experiments later when the experimental results come available. Although it should be noted that such a comparison will not be easy due to the differences in boundary conditions. Where the numerical codes can employ periodic boundary conditions assuming fully developed flow, the experiments certainly will not employ thermally developed flow. This would require a flow length of more than 260 hydraulic diameters, which is observed by [12] as the thermal development length of a 7 pin wire-wrapped sodium-cooled rod bundle.

### **2.1. Geometry and boundary conditions**

The 19 rods are arranged in a hexagonal lattice with a pin-to-pin center pitch of 8.4 mm. The external diameter of the pins is 6.55 mm and the internal diameter of the steel cladding is 5.07 mm. Each pin contains a wire spacer with a diameter of 1.75 mm and a wrapping pitch of 262 mm. This leaves a minimal area between the wire and the next rod of 0.1 mm. To facilitate meshing, fillets are introduced in the simulations between the rod and the wire instead of using point contacts. The radius of this fillet is chosen to be 0.25 mm to have a smooth transition between the wire and the rod which can be meshed in all different codes. The rod bundle is constrained by a hexagonal wrapper with a corner to corner distance of 45.43 mm. The orientation of the wire at the inlet has been selected in the way that at  $z=38\text{mm}$  the wire is in-line with the x-axis, which is consistent to the NACIE\_UP experiment. The rotation of the wire is counterclockwise in the positive z-direction. An overview of the geometry and the geometric properties is provided in figure I and table I.

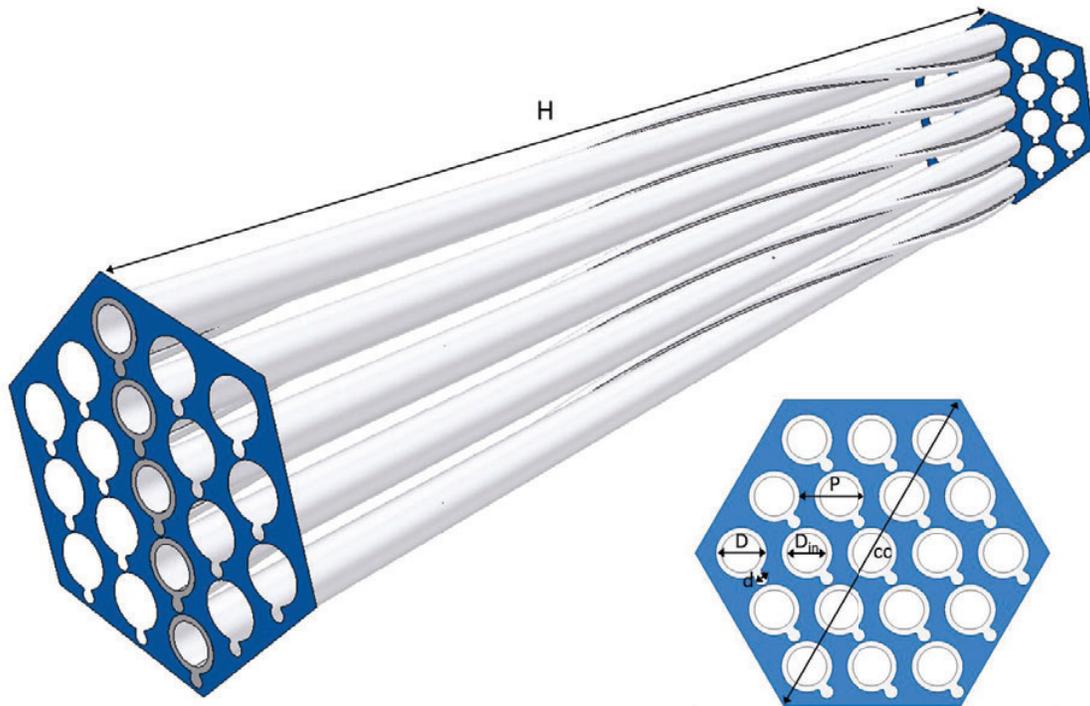


Figure 1: Overview of the geometry

Constant properties of the LBE are assumed, computed at the inlet temperature of 200 °C, based on the OECD/NEA handbook [9], in order to facilitate periodicity. The steel is also assumed to have constant properties, those of steel AISI 304. The Reynolds number based on the bundle hydraulic diameter is 30 000. A summary of the boundary conditions, which might be normalized in the computation, is provided in table II. The mean axial velocity and the increase of the average bulk temperature in 1 wire pitch, computed from the mass and heat balance, are 1.8 m/s and 51.8 K.

Table I. Geometric properties of the 19-pin wire-wrapped rod bundle

Part	Character	Size (mm)	Dimensionless size
Outer rod diameter	D	6.55	1 D
Inner rod diameter	$D_{in}$	5.07	0.774 D
Wire diameter	d	1.75	0.267 D
Fillet radius	r	0.25	0.038 D
Pin pitch	P	8.4	1.28 D
Wire pitch	H	262	40 D
Corner to corner distance hexagonal wrapper	cc	45.43	6.94 D
Hydraulic diameter	$D_h$	3.84	0.586 D

**Table II. Boundary conditions**

Boundary	Boundary condition	Value
Inlet	Mass flow rate	12.36 kg/s
	Reynolds number	$3.0 \cdot 10^4$
	Mean temperature	473.15 K
Inner diameter rod cladding	Heat flux	Total power 94.65 kW
Walls	Velocity treatment	No-slip wall
Inlet and outlet	Velocity	Periodic
	Temperature	Periodic

## 2.2. Computational methods

The reference data, provided by Argonne, are obtained in the spectral open-source code Nek5000. This code is developed within the SHARP suite: Simulation-based High-efficiency Advanced Reactor Prototyping. More information about the SHARP suite and the NEK5000 can be found in [8]. A preliminary Large Eddy Simulation (LES) is performed using a mesh consisting of 600 000 spectral elements or 300 000 000 points (see figure 2). A mesh improvement is foreseen by applying local refinement. Therefore the current reference LES results are referred to as preliminary LES results. A 7<sup>th</sup> order solver is applied for the continuity equation.



**Figure 2: A slice of the preliminary LES mesh**

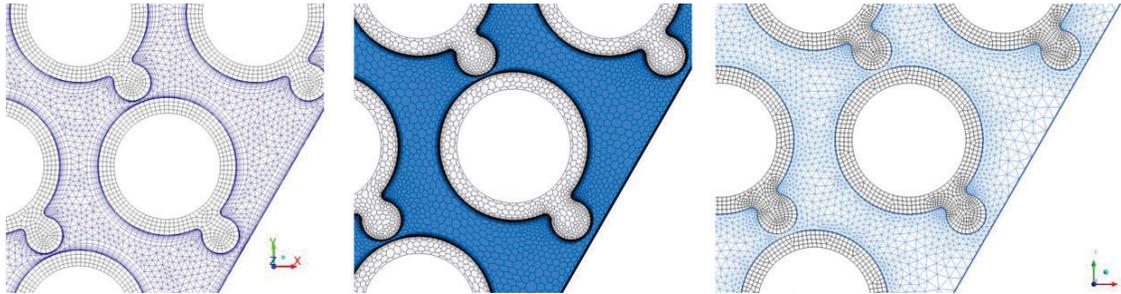
The participants to the benchmark performed Reynolds Averaged Navier-Stokes (RANS) simulations. Due to the smaller computational requirements, this method could provide a more pragmatic method to compute the thermal-hydraulics of a complete fuel assembly, multiple fuel assemblies or even a complete core. Therefore, the determination of the accuracy of the results obtained with RANS simulations compared to LES simulations is the purpose of this benchmark.

UGent used an undisclosed commercial code and created a finite volume mesh of 40 million cells (figure 3 left), consisting of tetrahedral cells in the bulk and a boundary layer of prismatic cells. The solids domain is meshed with hexagonal cells. The average  $y^+$  is 1. The  $k-\omega$  SST turbulence model is applied and all discretization schemes are second-order upwind.

NRG used the commercial finite-volume code Star-CCM+ 9.4 with a mesh of 48 million polyhedral cells in the fluid and 14 million polyhedral cells in the steel (figure 3 center). The fluid has a boundary layer of hexahedral cells. Also in the solid a small boundary layer has been applied in order to have a smooth transition in cell size between the solid and the fluid. The average  $y^+$  in the domain is 0.9. The

standard low Reynolds number  $k-\varepsilon$  turbulence model is applied with all  $y^+$  treatment and second-order upwind discretization schemes are used.

ENEA performed the RANS computations in the commercial software CFX version 15. A 81 million cells mesh is applied consisting of tetrahedral cells with a hexahedral boundary layer (figure 3 right). The  $k-\omega$  SST turbulence model is applied using second-order upwind discretization schemes.

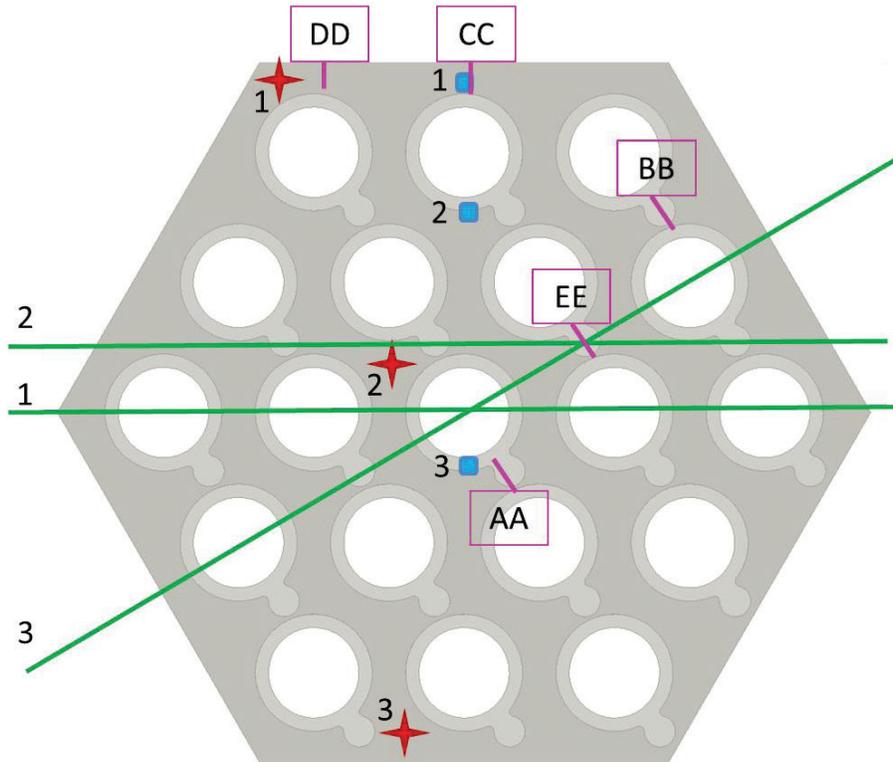


**Figure 3: Employed RANS meshes, UGent mesh (left), STAR-CCM+ mesh (center), CFX mesh (right).**

### 2.3. Benchmark comparison

Similar comparisons are conducted as in the first benchmark [8]. Obviously the comparisons had to be extended due to the larger amount of rods and the inclusion of the temperature. Four comparisons are distinguished:

- Velocity components ( $u,v,w$ ) and temperature on three streamwise lines in the center of different sub-channels (indicated by red stars (★) in figure 4). Three different types of sub-channels are selected: sub-channel 1 is a corner sub-channel, number 2 is a central sub-channel near the central rod and sub-channel 3 is an edge sub-channel.
- Velocity components ( $u,v,w$ ) and the temperature on Diag1, Diag2, and Diag3 (indicated by green lines (-) in figure 4) on five stream-wise normal planes spaced uniformly in  $z$  [for plane  $i$ , the axial height is  $z=i(H/5)$ ].
- Average transversal velocity (cross flow) on lines A-A, B-B, C-C, and D-D indicated by magenta lines (-) in figure 4 across the whole stream-wise direction. Data was compared across 200 lines per location, uniformly spaced in  $z$  (only one data point at the periodic boundaries is required).
- Temperature at the outside of the cladding (indicated by blue squares (■) in figure 4) at three lines in axial direction. 200 points are sampled uniformly at each line.



**Figure 4. Schematic overview of benchmark comparison strategy, showing the inlet plane. The red stars (★) indicate the center of three sub-channels, the green lines (-) indicate three diagonals, the small magenta lines (-) with letters indicate five axial planes and three axial lines at the cladding are indicated by blue squares (■).**

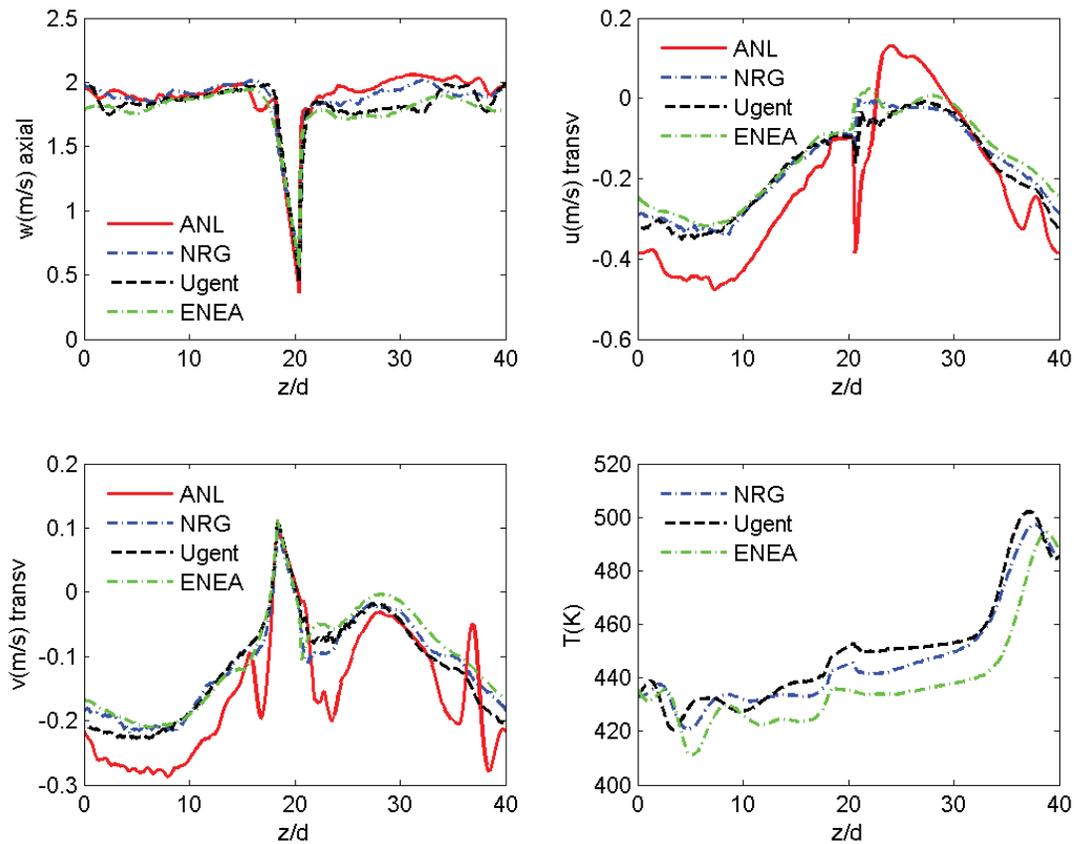
### 3. RESULTS

This section provides two types of results: the comparison between the RANS contributions with the preliminary LES results, and a comparison of the RANS results where the LES data are not available yet. The error of the RANS results with respect to the LES results is computed as follows:

$$E = \frac{\sqrt{\frac{1}{N} \sum_{i=1}^N (f_i - f_i^{LES})^2}}{F}$$

with  $N$  the number of points for the comparison,  $f_i$  the value of the function that is being compared and  $F$  the normalization. All velocity results are normalized by the mean axial velocity. The temperatures are normalized with  $\Delta T$ , which is the mass flow averaged bulk temperature increase over 1 wire pitch.

### Subchannel 1



**Figure 5. Comparison sub-channel 1.**

The comparison of the velocity components in corner-sub-channel 1 is provided in figure 5, where a wire crosses at  $z/D = 20$ . The same trends are observed in the LES as in the RANS, although the dips and peaks in the secondary velocities are smaller in the RANS. The normalized RMS error is similar for all three RANS computations, as can be seen in Table III. The axial velocity component has an error below 9% and the normal velocity components are below 7% error. In the comparison of the RANS temperature results it is observed that the peaks are at slightly different axial locations. This might be due to different meshing strategies and different methods of achieving thermal periodicity in the various CFD codes.

The reduction of the peaks and dips by the RANS method is also observed in the diagonals. An example of the comparison is provided by the second diagonal at  $z/d = 32$  in Figure 6, where four crossing wires can be observed by the sharp peaks or dips. Overall, the axial flow component has an error below 12.5% and the transversal flow components below 4%. The temperature predictions of the RANS computations are quite similar.

The RANS models predict the transversal velocities well (see Figure 7; the wire crosses at  $z/d = 0, 20$  and  $40$ ). The velocity peaks at the small gap of the wire crossing is different, were the results of ENEA are closest to the reference data. This difference could be enhanced by the reduction of the plane through which the transversal flow is flowing, making the comparison more sensitive to small differences in the numerical representations of the geometry and meshing differences. The normalized error is provided in table III, being below 3%.

Finally the normalized cladding temperature of figure 8 shows a reasonable agreement between the RANS computations of UGent and NRG and ENEA.

line 2 z over d=32

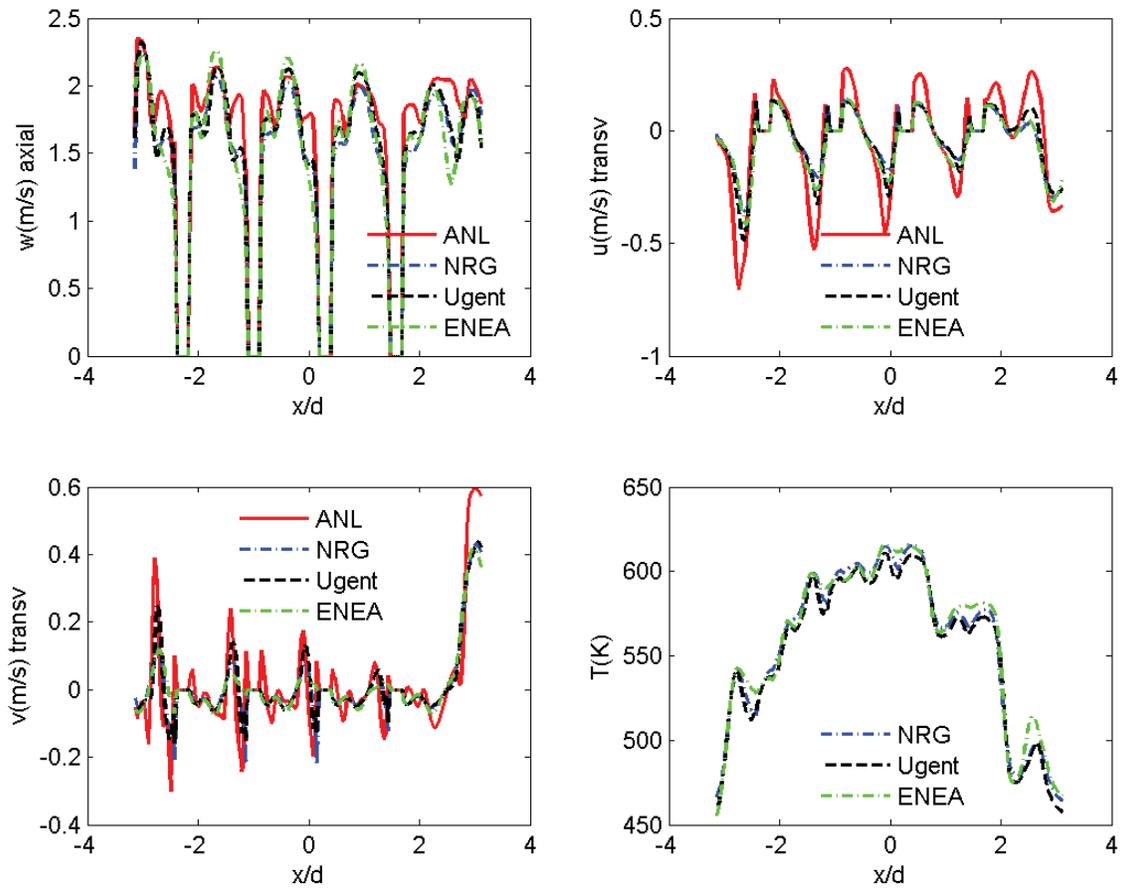


Figure 6. Comparison of the results at diagonal 2 at  $z/d = 32$ .

### Transversal flow through AA, BB, and EE

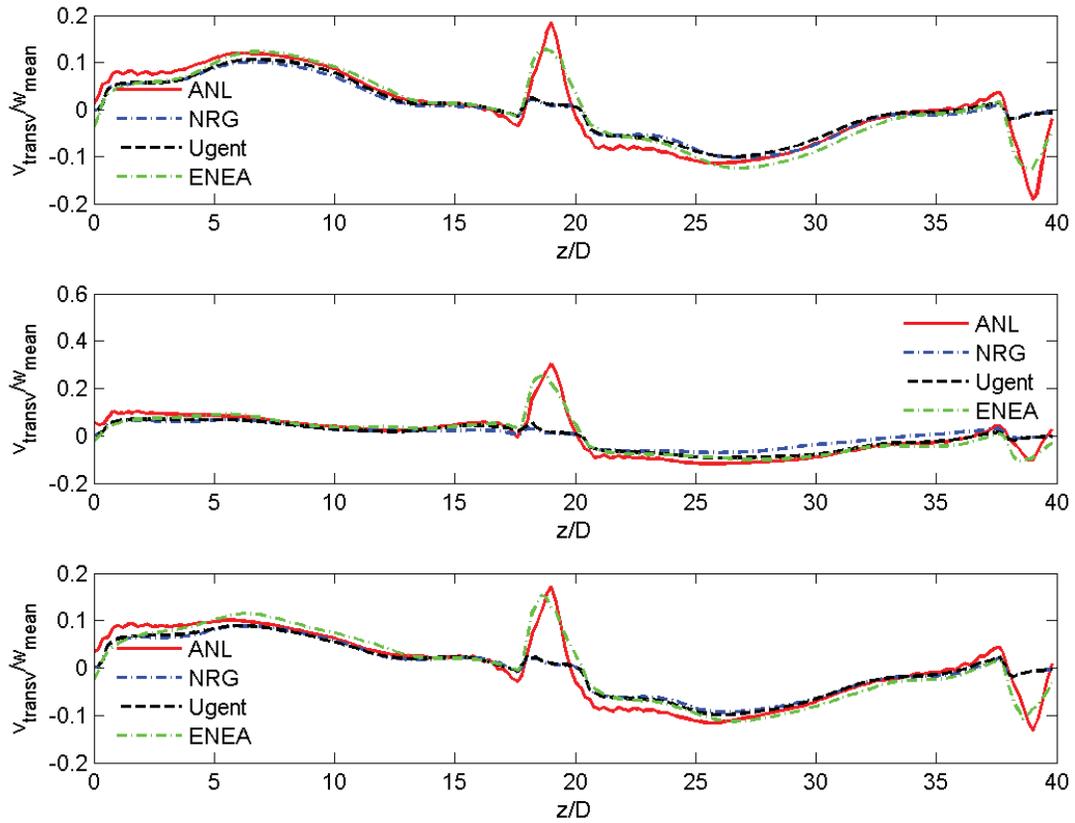
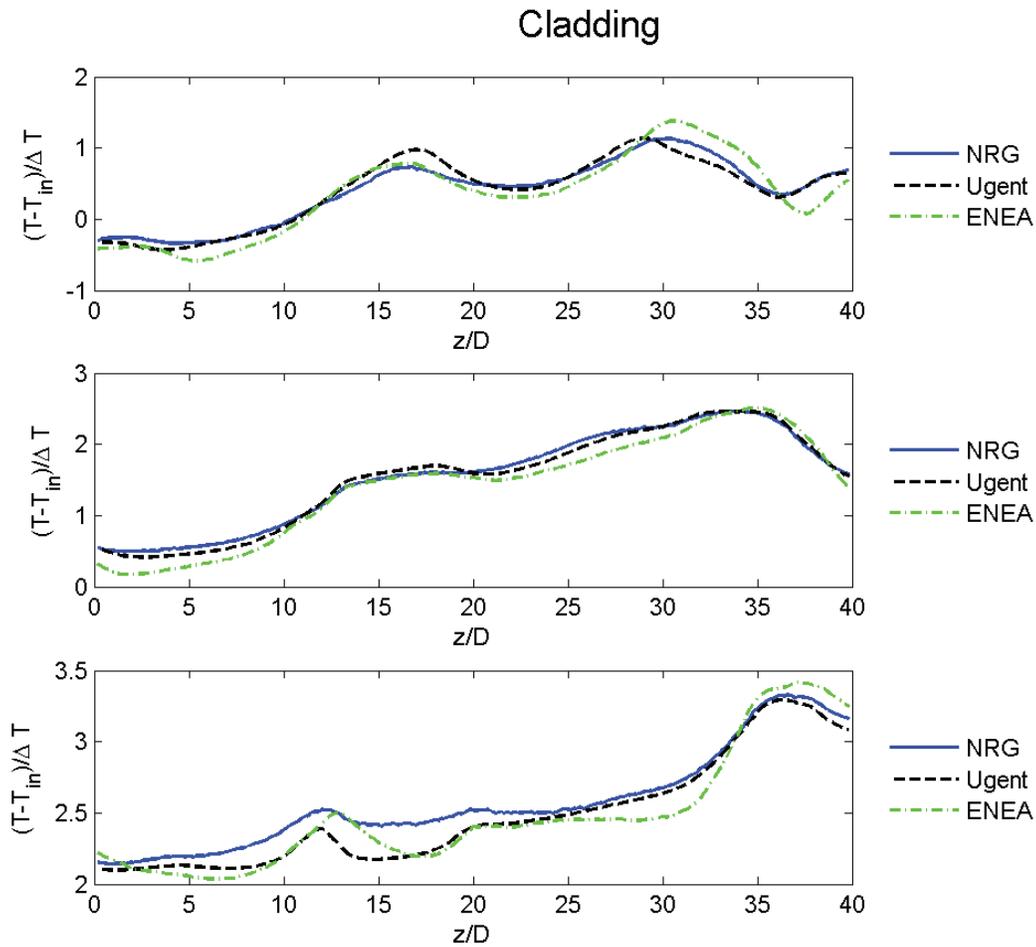


Figure 7. Normalized transversal velocity through planes AA (top), BB(middle) and EE (bottom).



**Figure 8. RANS results of the cladding temperature at lines 1 (top), 2 (middle) and 3 (bottom).**

As mentioned above, table III summarizes the error of the RANS results with respect to the reference LES, normalized by the mean axial velocity (1.8 m/s) or the temperature increase over 1 wire pitch (51.8 K). The error of the RANS normal velocity components is below 7%. The axial velocity components are modelled with an error below 12.5%. The errors are similar for all three RANS computations.

**Table III. RMS difference between the RANS and the LES results, expressed as percentage of the mean axial velocity (1.8 m/s) or the average bulk temperature increase over 1 wire pitch (51.8 K).**

Comparison	Variable	NRG	UGent	ENEA
Subchannel 1	u	5.9	5.5	6.8
	v	3.5	3.3	4.0
	w (axial)	4.4	7.3	8.3
Subchannel 2	u	4.9	4.2	4.2
	v	4.5	4.1	3.7
	w (axial)	6.1	6.9	8.8
Subchannel 3	u	4.0	3.0	5.5
	v	3.8	3.4	3.6
	w (axial)	5.1	5.4	6.6
Diagonal 1	u	1.7	1.5	1.8
	v	3.2	3.0	3.5
	w (axial)	10.0	9.8	12.3
Diagonal 2	u	3.9	3.3	3.7
	v	3.1	2.9	3.2
	w (axial)	8.4	9.3	11.8
Diagonal 3	u	2.9	2.6	2.6
	v	3.1	2.9	3.1
	w (axial)	6.9	7.2	9.7
Transversal velocity aa	Transversal velocity	2.1	2.0	1.1
Transversal velocity bb	Transversal velocity	2.9	2.6	1.2
Transversal velocity cc	Transversal velocity	2.3	2.2	2.2
Transversal velocity dd	Transversal velocity	2.5	2.5	2.3
Transversal velocity ee	Transversal velocity	1.7	1.7	1.1

#### 4. CONCLUSIONS & OUTLOOK

The thermal-hydraulics of a 19-pin wire-wrapped rod bundle representative for a MYRRHA fuel assembly is assessed in this benchmark. All trends are well captured by the RANS models. The error of the RANS transversal velocity components is below 7%. The axial velocity components are modelled with an error below 12.5%. The errors are similar for all three RANS computations.

A more detailed comparison with an improved LES computation and a comparison of the thermal field of the LES computation are foreseen. Besides, experimental data of the temperature will be produced in the NACIE-UP facility at ENEA, so a second thermal verification can be envisaged.

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