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## Towards validated prediction with RANS CFD of flow and heat transport in a wire-wrap fuel assembly



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### ABSTRACT

Liquid metal fast reactors (LMFRs) are foreseen to play an important role in the future of nuclear energy, thanks to their increased fuel utilization and safety features profiting from the optimal heat transfer performance of the metallic coolants. Accurate thermal-hydraulic analysis of their fuel assemblies, typically employed with wire-wraps as spacers, is recognized as a crucial scientific and engineering contribution to support the deployment of such technology. This challenges the modeling and simulation community.

To this aspect, various reference databases (both experimental and numerical) for different wire-wrapped fuel assembly configurations have been created recently and are being used for validation of engineering simulation approaches based on Reynolds Averaged Navier Stokes (RANS) modelling. These databases include:

- 7-pin rod bundle: A detailed experiment with Particle Image Velocimetry (PIV) is performed. In order to allow accurate measurements of the flow topology, a matched-index-of-refraction technique was used employing water as working fluid.
- 19-pin bundle: A series of experiments is performed covering a wide range of Reynolds and Peclet numbers as well as thermal powers. The experiments use liquid lead-bismuth eutectic as working fluid. The measurements include pressure drop and local temperatures.
- 61-pin rod bundle: This large eddy simulation including conjugate heat transfer from the pin cladding to the coolant allows to bridge the gap from small bundles (less than 37 pins) to large bundles (more than 37 pins). In literature, a fundamental different behavior has been observed for small bundles compared to large bundles.
- 127-pin bundle: Isothermal experiments using lead-bismuth eutectic characterizing pressure drop are performed on a full scale fuel assembly representative for the MYRRHA reactor.
- Infinite pin bundle: This reference quasi-direct numerical simulation profits from periodicity in all directions. It provides a detailed view into the flow field and in addition reveals details of the heat transfer from the rod bundle into the flow.

Reference databases aim to serve the nuclear scientific community to validate engineering simulation approaches. The paper will introduce these reference databases, and how they have been used to validate RANS based turbulence modelling approaches within a mainly European context.

### 1. Introduction

Nuclear energy production world-wide contributes to the world energy production as one of the main low CO<sub>2</sub> emitting energy sources. Given the current reserves of uranium in the world and their application in the current light water reactors, it is predicted that the uranium reserves should be sufficient for the coming 100–150 years. In order to make nuclear energy production more sustainable in the future, a switch to fast neutron reactors will extend this time horizon for one or two centuries significantly. Among the fast neutron reactor designs, the

ones cooled with liquid metals are most mature. In fact, a number of sodium-cooled fast reactors and a few lead-bismuth cooled reactors have been or are operational worldwide. Accurate thermal-hydraulic analysis of their fuel assemblies, mostly employed with wire-wraps as spacers, is recognized as a crucial scientific and engineering contribution in order to support the deployment of such technology. This challenges the modeling and simulation community as well as experimentalists.

As explained in Roelofs et al. (2018), for the design and safety assessment of such wire-wrapped fuel assemblies, from the thermal-

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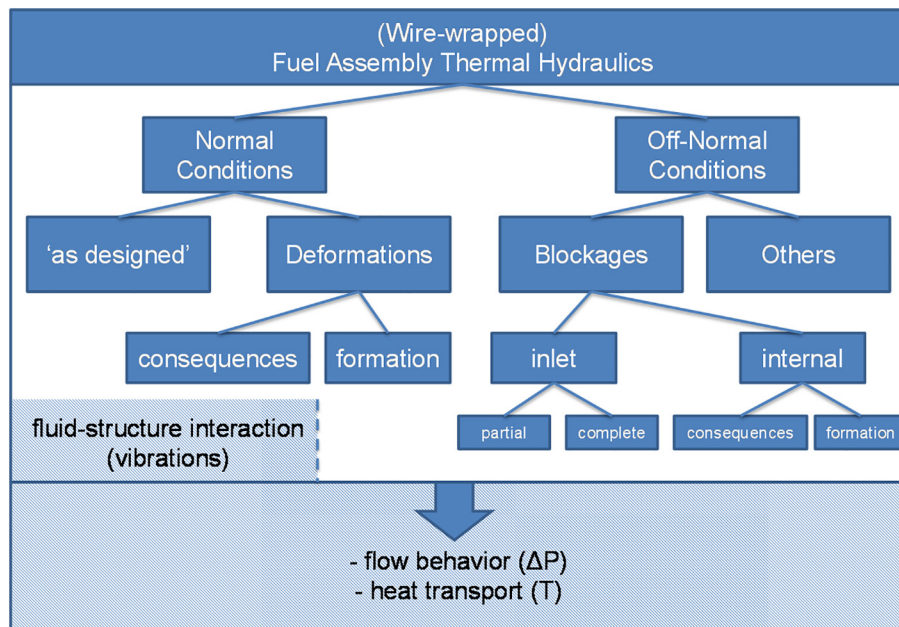


Fig. 1. Issues to be analyzed in the field of wire-wrapped fuel assembly thermal-hydraulics (Roelofs et al., 2018).

hydraulic point of view many issues need to be addressed. It typically starts from the assessment of flow and heat transfer (mostly pressure drop and maximum temperatures or temperature gradients) under normal operating conditions for fuel assemblies as they are designed. Most of the existing publications to date, especially in the field of CFD simulations, are limited to this. However, it may be clear from Fig. 1 that, although this is an important issue to address, there is a lot more to take into account. Under operational condition, a careful check should be made towards the possible occurrence of vibrations in the fuel assembly. But additionally, it should be realized that fuel assemblies will deform, even under operational conditions. Such deformations may be caused by manufacturing issues (e.g. pre-stressing the wires) or e.g. by expansion due to heating up to operational temperature from ambient conditions. From that point of view, analyses are needed to assess the formation and consequences of such deformations on the flow and heat transport. However, apart from the normal operating conditions, also situations of off-normal conditions need to be analyzed. Most of these studies concern in one way or the other the consequences of blockages. Blockages can be formed at the inlet of a fuel assembly or internally within the pin bundle. For the case of inlet blockages, the case of partial inlet blockages needs to be analyzed as well as the case of complete inlet blockages.

The validation strategy of engineering CFD simulations for wire-wrapped fuel assemblies, typically Reynolds-Averaged Navier Stokes (RANS) simulations, is based on the triangle of CFD methodologies which is schematically indicated in Fig. 2. For validation, experimental data is typically used as reference. However, experiments have practical limitations, especially when liquid metals are involved. Apart from that, computer capacities are increasing. Therefore, high-fidelity numerical simulations in which the numerical and modelling errors are minimized (so-called Direct Numerical Simulations (DNS)) are used as reference data. One should however realize that such simulations are restricted to small size domains and relatively low Reynolds numbers as the computational efforts required are huge. A DNS methodology can only be applied at sub-channel level and for idealized conditions. When switching from DNS to Large Eddy Simulation (LES), larger domains are feasible, but this comes at the cost of a loss in accuracy which in principle should be determined first. And even with the use of LES, one is restricted to limited sized computational domains, unless High Performance Computing (HPC) is applied. The use of DNS (or a

alternatively LES) as reference data is extremely valuable, since in contrast to experimental data, the boundary and initial conditions are well defined and the analyst has in principle access to all locations of the flow and temperature field at every time step of the simulation. Ideally, validation of engineering CFD methodologies should be based on a combination of comparisons to experimental and numerical reference data. The experimental data will allow to compare to 'reality' but are limited in resolution and measurement possibilities and include uncertainties in geometry and boundary conditions, whereas the numerical reference data will allow to have access to well defined data with respect to geometry and boundary conditions and, in principle at every location in the domain without restrictions, but preferably numerical reference data should be compared as well to experimental data.

Apart from that, it is important to realize that validation can be split into validation of the hydraulic behavior on the one hand (i.e. the momentum field characterizing friction, pressure drop and velocity field) and the validation of the thermal-hydraulic behavior on the other hand (i.e. the thermal field characterizing local temperatures and heat fluxes). The following two chapters will provide examples of validations performed at sub-channel level and at fuel assembly level (see Fig. 2) for the hydraulics as well as thermal-hydraulics validation of wire-wrapped fuel assemblies at NRG in the Netherlands using primarily European reference data. For an extensive overview on experimental and numerical data available internationally, the reader is referred to Roelofs (2019) or Roelofs et al. (2019). In the latter publication, an attempt is made to collect available comparisons from all over the world between reference data on wire-wrapped fuel bundle data at various sizes and RANS simulations. Validations at core level remain difficult because of the lack of availability of reference data, both experimental as well as numerical. At the level of the core, one typically has to rely on the validation performed at fuel assembly level.

An important feature to consider was identified by Brockmeyer et al. (2017). They observed a significant difference in behavior between 'small bundles' (less than 37 pins) compared to 'large bundles' (more than 37 pins). For correctly mimicking the behavior in a full size bundle (typically 127 pins or more), they recommend to use at least 37 pin bundles, where the effect of the fuel assembly casing in the central sub-channels is negligible. Nevertheless, smaller bundles are considered useful, especially with respect to measurement accuracy and

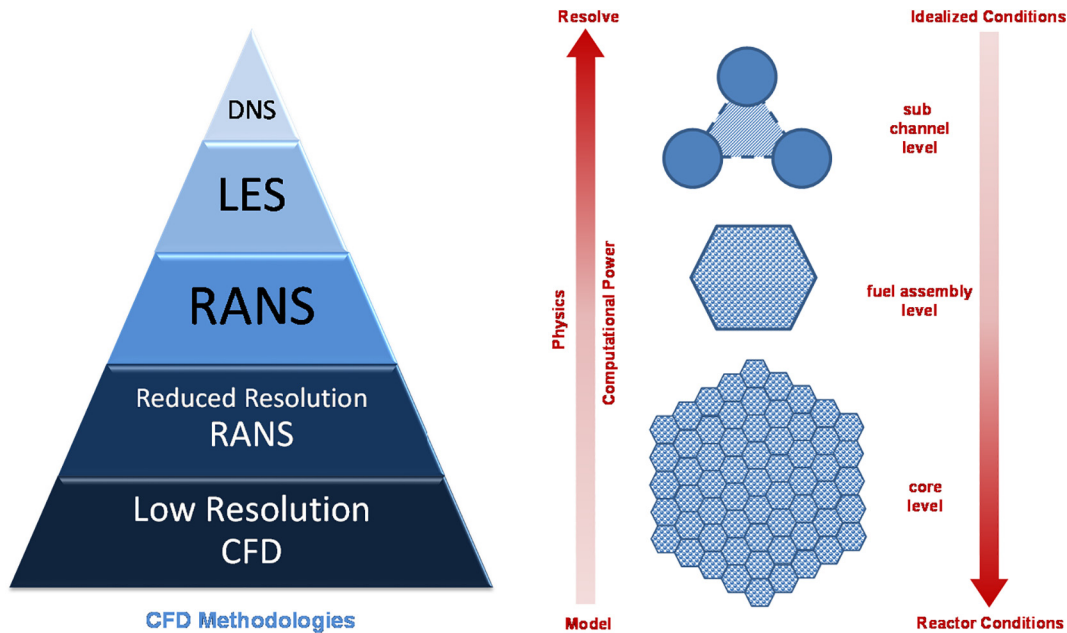


Fig. 2. The triangle of CFD methodologies and its relation to fuel assembly thermal hydraulics (Roelofs et al, 2018).

affordability (both budget-wise as computation-wise) for the validation of numerical methodologies

In all following sections, the accuracy is determined as follows:

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

with  $N$  the number of points for the comparison,  $f_i$  the value of the function that is being compared,  $f_i^{ref}$  the reference value that is being compared to, 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. Note that, using the latter normalization for temperature, increasing the length of the simulated domain will reduce the difference between model and reference data. For the applications presented in the current paper which are mostly related to a single or just a few wire pitches, this is supposed to have limited influence.

The following sections deal with respectively the validation based on 7-pin, 19-pin, 61-pin, 127-pin, and infinite pin bundle data. Each section is subdivided in a short explanation about the data production program and a summary of the numerical program highlighting the validation of numerical engineering methods achieved. Finally, section 7 presents the conclusions, summarized in a table showing the validation efforts and achieved accuracies.

## 2. 7-Pin bundle

A limited sized 7-pin bundle is often studied because experimentally this is less costly than larger bundles and allows better access to the central channels. Apart from that, a 7-pin bundle is also often studied because numerically it requires modelling of a smaller domain and therefore allows to use required mesh refinements especially near walls leading to better accuracy. Finally, smaller computational domains are less costly and allow sensitivity studies.

### 2.1. Data production program

Merzari et al. (2016) presented an LES simulation for a 7-pin bundle which was used as a benchmark to test RANS turbulence models as no suitable experimental dataset was available at that moment. Although the LES was carried out with great care, numerically some geometrical

approximations had to be made and as explained before an LES always brings modelling uncertainties. Therefore, more recently, a matched-index-of-refraction (MIR) experiment was designed in the Netherlands at the university of Delft. The experimental set-up is called SEEDS-2 (SEven rods Experiment in Delft for SESAME number 2). This experiment aims at the creation of accurate measurement data using Particle Image Velocimetry (PIV) and Laser Doppler Anemometry (LDA) optical techniques. In the experiment (see Fig. 3) the 7 pins in the test section were created of Fluorinated Ethylene Propylene (FEP), a material also used by Mahmood (2011) with the same refractive index of water (Bertocchi et al., 2018), whereas the wires were made of metal. More details of the test section are described by Bertocchi and Rohde (2016). The experimental data was obtained through PIV measurements which were independently checked by LDA measurements. Typically, measured data comprises velocity components as well as their fluctuations for a range of Reynolds numbers varying from about 4000 to 15,000. Fig. 3 shows examples of measurement data obtained in SEEDS-2. The dark blue sections indicate regions where measurement data is not available because of reflections of the wire which prohibit sufficiently accurate measurements.

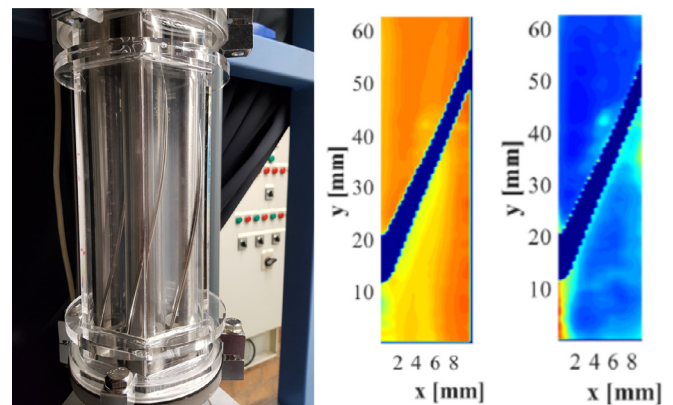


Fig. 3. MIR experimental set-up and an example of axial velocity and velocity fluctuations measurements.

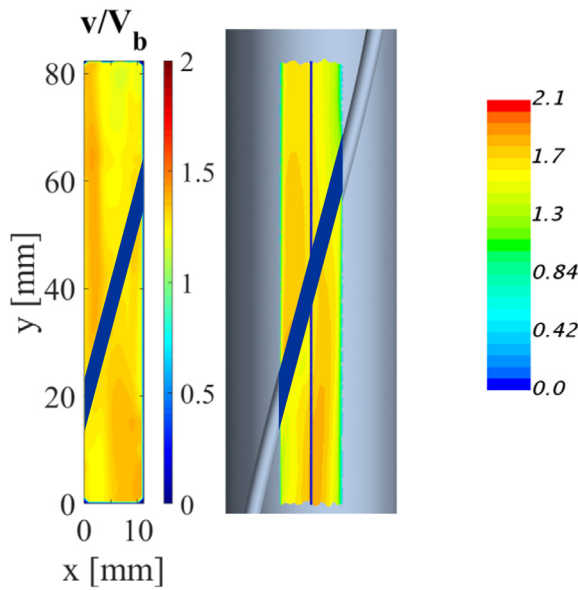


Fig. 4. Qualitative comparison of experimental (left) and numerical (right) data for the 7-pin MIR experiment.

2.2. Numerical program

The numerical benchmark reported by Merzari et al. (2016), comprised 2 isotropic (realizable  $k-\epsilon$  and SST  $k-\omega$ ) and 1 anisotropic (cubic  $k-\epsilon$ ) wall resolved RANS models. Mean velocities were predicted within 10% and in many cases within 5% with all applied turbulence models and a wall resolved mesh. It was concluded that the application of an anisotropic model does not bring significant added value for this 7-pin wire-wrapped assembly. Furthermore, it was underlined that high-resolution experimental investigations are necessary for further modelling development.

With respect to the simulations of the matched-index of refraction experiments, the data analysis is still ongoing. The simulations performed use a wall resolved mesh of about 29 million cells. Uncertainties in measurements and simulations are currently being addressed to allow fair quantitative comparison of the data. Numerically, the isotropic SST  $k-\omega$  is used as well as the anisotropic cubic SST  $k-\omega$  and RSM-EB turbulence models. Qualitatively, the same behaviour can be identified in experiments and simulations as shown in Fig. 4. For comparison, also in the simulation results, the data coinciding with the wire position are omitted. Fig. 5.

3. 19-Pin bundle

In Europe, two independent sets of experiments on 19-pin heated bundles in liquid metal were performed by Di Piazza et al. (2016) and Pacio et al. (2016). The first one focused on natural convection conditions, while the second one focused on forced convection conditions.

3.1. Data production program

The geometry and operating conditions of temperature, flow velocity and power density of the experiment in the KALLA facility described by Pacio et al. (2016) are representative for the fuel assemblies envisaged for the lead-bismuth cooled MYRRHA reactor under design in Belgium. For this experiment, an extensive test matrix comprising of more than 30 experimental runs was analysed. The Reynolds number varies from 14 000 to 48 000 while the Péclet number varied from 400 to 1500. Thermal power was supplied up to 295 kW at an inlet temperature of 200 °C. Dealing with liquid metal, no velocity measurements were performed. However, both pressure drop and heat transfer are measured and where possible compared to available correlations. Specifically, detailed cross-sectional temperature distributions at three selected axial positions are obtained. These data serve as validation data for CFD.

Also the geometry and operating conditions of the experiment in the NACIE facility described by Di Piazza et al. (2016) are representative of the a fuel assembly envisaged for MYRRHA. For the NACIE experiments, the Reynolds number was varied from 1000 to 14 000 while the Péclet number varied from 25 to 250.

3.2. Numerical program

The 19-pin heated experiments in the KALLA facility reported by Pacio et al. (2016) were used to validate RANS modelling. This effort is described in Pacio et al. (2017). There, it is shown that the wall resolved RANS model consisting of about 200 million cells can predict the pressure drop at similar accuracy as described earlier for Merzari et al. (2016), Doolaard et al. (2015), and Kennedy et al. (2015). The main focus for validation was on temperatures and heat transport. Fig. 6 (top) shows an example of temperature predictions for the experiments of Pacio et al. (2016) leading to the conclusion that heat transfer (Nusselt number) can be predicted within 12% (Pacio et al., 2017) using a wall resolved mesh and an SST  $k-\omega$  model with a default constant turbulent Prandtl number of 0.9. A future assessment of the impact of using more advanced turbulent heat flux models as described in Roelofs et al. (2015) and more recently in Shams et al. (2019) is recommended.

With respect to the NACIE experiments reported by Di Piazza et al. (2016), the RANS simulations of NRG shown in Fig. 6 (bottom) used a wall resolved mesh of about half the size of the mesh used to simulate

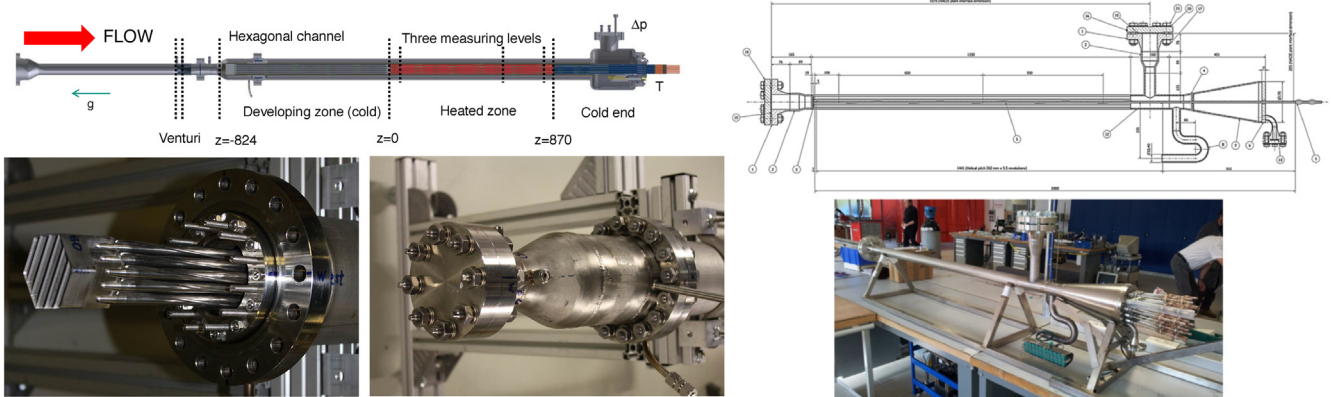


Fig. 5. Experimental set-up for the lead-bismuth 19-pin experiments in the KALLA facility (Pacio et al., 2016) and the NACIE facility (Di Piazza et al., 2016).

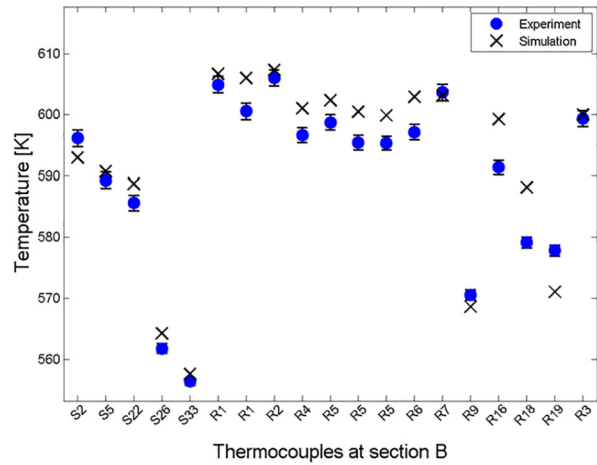
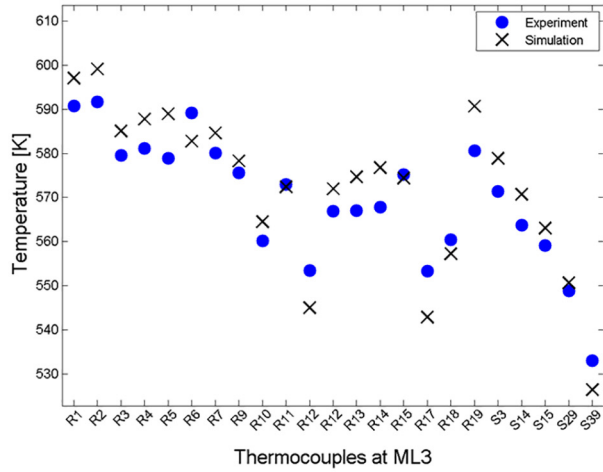
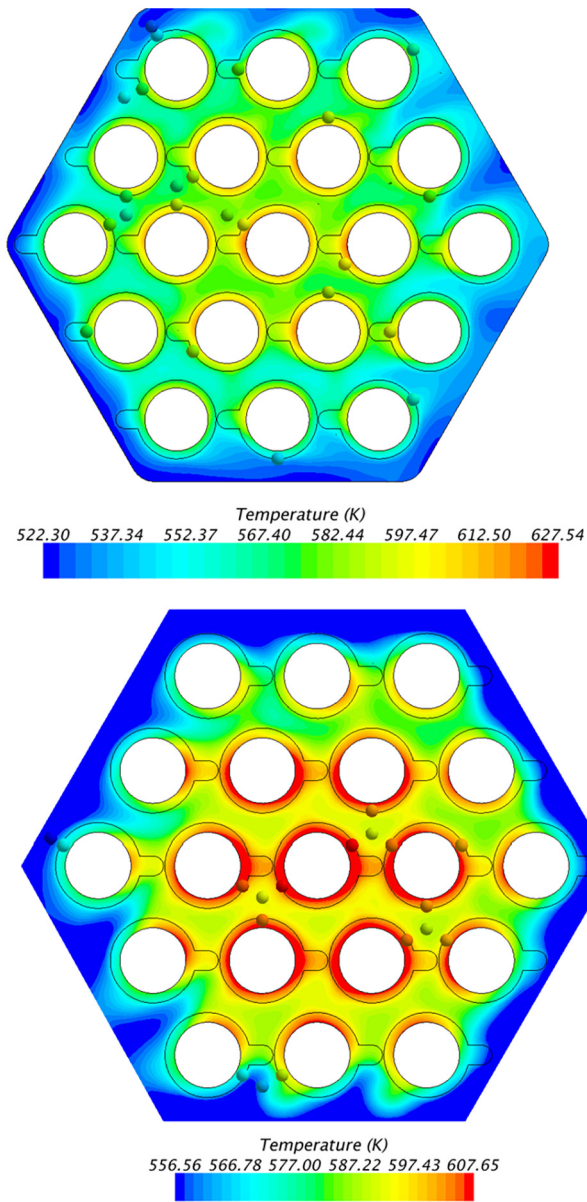


Fig. 6. Simulated contours of temperature in the KALLA (top) and NACIE (bottom) 19-pin bundle experiments with positions of thermo-couples indicated (left) and a comparison of thermo-couple readings from simulation and experiment (right).

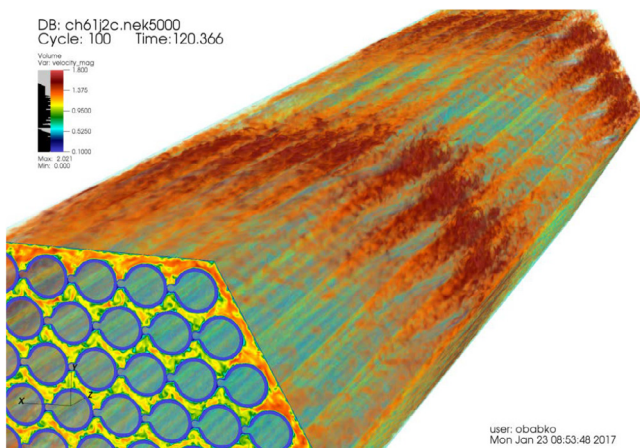


Fig. 7. Volume rendering of the LES simulation for instantaneous axial velocity at  $Re = 15,000$  (Mays, 2017).

the experiments in the KALLA facility, i.e. 100 million cells. This was possible as the flow rates in NACIE are considerably smaller. Again the SST  $k-\omega$  model was used. Simulation results for the temperature difference normalized by the difference between the bulk and inlet temperature were within 10% accuracy.

#### 4. 61-Pin bundle

In the US, a validation program for wire wrapped rod bundles was established based on a 61-pin bundle. This comprised a MIR experiment (Goth et al., 2018a) and Nguyen et al. (2017, 2018), a heated experiment (Mays et al., 2016) and supplementary LES (Obabko et al., 2016). Through a US-EU collaboration, the LES data has been made available to EU partners in the frame of the SESAME project.

##### 4.1. Data production program

As mentioned before, the LES of Obabko et al. (2016) was related to the MIR experiments described by Goth et al. (2018a) and Nguyen et al.

(2017, 2018). A comparison of the LES results (see Fig. 7) to the experimental data in an interior sub-channel for a Reynolds number of 19 000 is presented by Goth et al. (2018b). They conclude that the shape and magnitude of the mean vertical velocity component is in good agreement with maximum relative errors less than 10% until the sub-channel walls are approached. Next to that, they claim that the shape and magnitude of the mean horizontal velocity components are in satisfactory agreement. While friction data generated in the 61-pin bundle (Vaghetto et al., 2018) have been compared with RANS simulations but not yet published, this is still an integral component of the data production program.

#### 4.2. Numerical program

Validation of RANS for the 61-pin bundle described before was performed based on comparison with the LES data presented by Goth et al. (2018b). To allow a good quality mesh in LES, it was decided to slightly flatten the wire near the adjacent pin as described in Goth et al. (2018b). To avoid any uncertainties in geometric modelling, the RANS model was based on the LES model using exactly the same geometry flattening the wire near the adjacent pin. RANS simulations were performed using the isotropic SST  $k-\omega$  turbulence model and the anisotropic cubic SST  $k-\omega$  model. Results indicate good comparison between LES and both RANS simulations as shown in Fig. 8 in which the anisotropic model shows slightly better performance for simulation of axial velocity. In addition, pressure drops predicted with RANS are within 5% of the pressure drop calculated in the LES simulation. Quantification of the further differences between LES and RANS is still in progress.

### 5. Full scale 127-pin bundle

Not many data are available on full scale bundles. Nevertheless, eventually the full scale bundle is what all the validation work on smaller scaled bundles is aiming at.

#### 5.1. Data production program

One of the few datasets for a full scale lead-bismuth eutectic (LBE) cooled bundle is presented by Kennedy et al. (2015). The experiment was conducted in order to characterize the pressure losses in a MYRRHA fuel assembly. These pressure losses dominate the overall primary system pressure loss and so knowledge of the coolant pressure drop across the fuel assembly is crucial to determine the primary pump design dimensions and specifications during normal operation. Furthermore, knowledge of the pressure loss characteristics at low flow

rates will allow designers to evaluate the possibility of passive decay heat removal. Therefore, an experimental campaign was setup at SCK-CEN to perform hydraulic testing of a full-scale mock-up (see Fig. 9) of a MYRRHA fuel assembly in the large-scale COMPONENT Loop Testing (COMPLOT) LBE facility at SCK-CEN.

The total volumetric flow rate through the fuel assembly test section is measured by means of a vortex flowmeter. The temperature of the LBE is measured by means of two temperature sensors, mounted upstream and downstream of the test section, with the thermowell probes positioned in the centre of the piping. The fuel assembly total pressure drop and the pressure drop across specific sections of the fuel assembly, such as the fuel pin bundle and the inlet and outlet nozzles, are measured differential pressure transmitters. More information on the instrumentation and measurement accuracy can be found in Kennedy et al. (2015).

#### 5.2. Numerical program

Kennedy et al. (2015) present a comparison of the pressure drop prediction in a full scale numerical pre-test RANS model, as depicted in Fig. 10, employing a mesh of 11 million cells. This pre-test RANS model applying an isotropic SST  $k-\omega$  turbulence model and a non-wall resolved (reduced resolution) mesh gave predictions of the pressure drop and friction factor with an accuracy of about 12% compared to the experimental values. The simulation also allowed to assess the temperature distribution in a heated bundle. To this purpose the heating profile provided by the designers was applied on an individual pin basis. However, the experiment was isothermal, so a comparison with experimental data can't be made and therefore results of this exercise are not shown here.

### 6. Infinite-pin bundle

#### 6.1. Data production program

Experimentally, the validation of the velocity and pressure field (hydraulics) in a wire-wrapped fuel assembly mostly relies on the similarity of the behavior in transparent fluids like water or air, and liquid metals. In recent years, matched-index of refraction (MIR) techniques have been applied for obtaining relevant experimental data as explained before. Such techniques allow to minimize the measurement errors in optical techniques caused by variations in refraction index by matching the refraction index of the transparent material used and the transparent fluid. However, complementary insights can be gained by performing (quasi) DNS simulations. Such simulations allow in

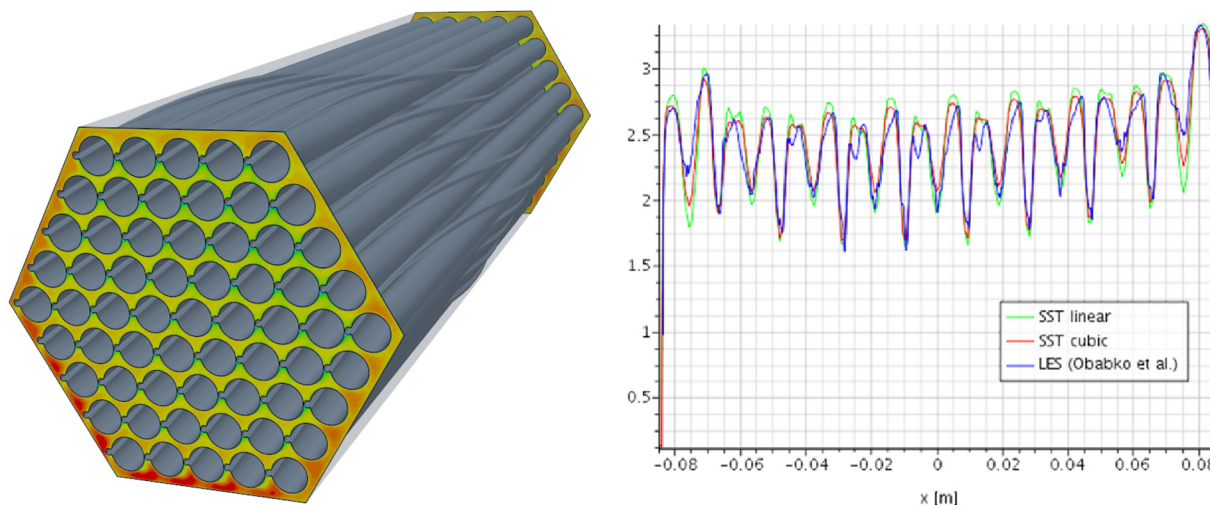


Fig. 8. RANS simulation of the 61-pin bundle and comparison of axial velocity with the reference LES data from the simulation presented by Goth et al. (2018b).



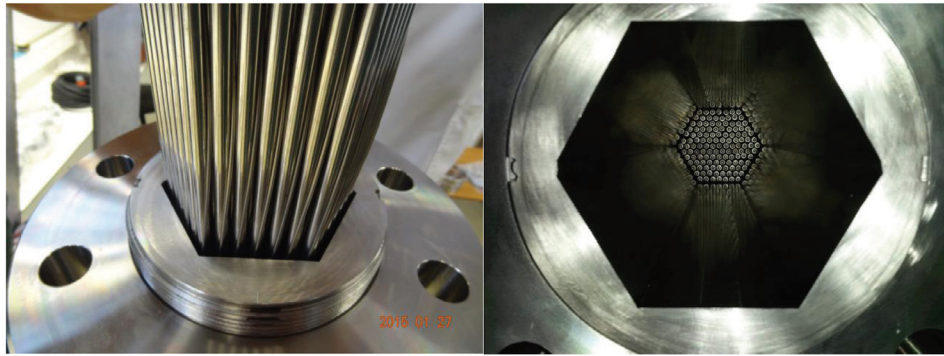


Fig. 9. The 127-pin MYRRHA fuel assembly mock-up in the COMPLIT loop (Kennedy et al., 2015).

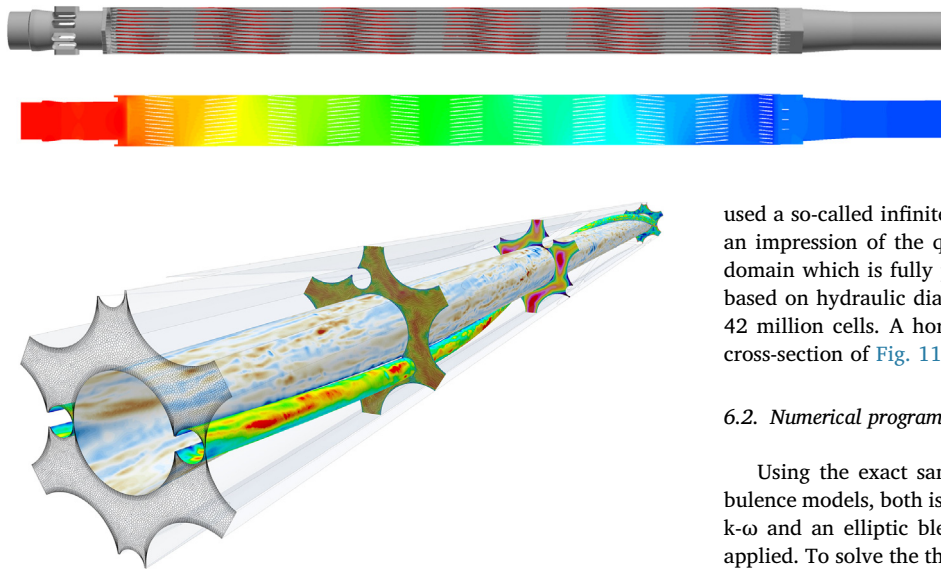


Fig. 10. Geometrical model of a MYRRHA 127-pin fuel assembly (top) and the pressure distribution (bottom).

Fig. 11. Impression of the quasi DNS performed on an infinite pin bundle.

principle access to all parts of the geometrical domain while the exact geometry that is applied is known without any uncertainties due to construction tolerances. Another advantage of such (quasi) DNS simulations is the fact that apart from the velocity field, also the temperature field can be analysed simultaneously which is hardly possible experimentally. As such, these kind of simulations are extremely valuable for validation of RANS approaches. However, due to the huge computational costs and the limitations in computer power, simulations are restricted to relatively small domains. Therefore, Shams et al. (2018)

used a so-called infinite bundle to create reference data. Fig. 11 shows an impression of the quasi DNS performed on an infinite pin bundle domain which is fully periodic in all directions at a Reynolds number based on hydraulic diameter of about 7000. The mesh contains about 42 million cells. A horizontal plane of the mesh is shown in the left cross-section of Fig. 11.

### 6.2. Numerical program

Using the exact same geometry as in the quasi DNS, various turbulence models, both isotropic (SST  $k-\omega$ ) and anisotropic (i.e. cubic SST  $k-\omega$  and an elliptic blending Reynolds stress model (EB-RSM)), were applied. To solve the thermal field a constant turbulent Prandtl number was used. Simulations revealed no difference between the use of the default value of 0.9 and a value of 2 typically employed for liquid metals based on Duponcheel et al. (2014). The RANS simulations show an accuracy in mean stream-wise velocity and temperature of within 5% for the anisotropic models and within 10% for the isotropic models while the mesh size is about 1/3 and the computational effort less than 1000 times smaller compared to the quasi-DNS. Finally, promising results are obtained for the turbulent kinetic energy and the Reynolds stresses, especially by the RSM-EB which is capable of reproducing quite well the peaks close to the walls. Fig. 12 shows an example of profiles for mean axial velocity (left) and mean temperature (right) along the line indicated in the picture of the instantaneous quasi DNS

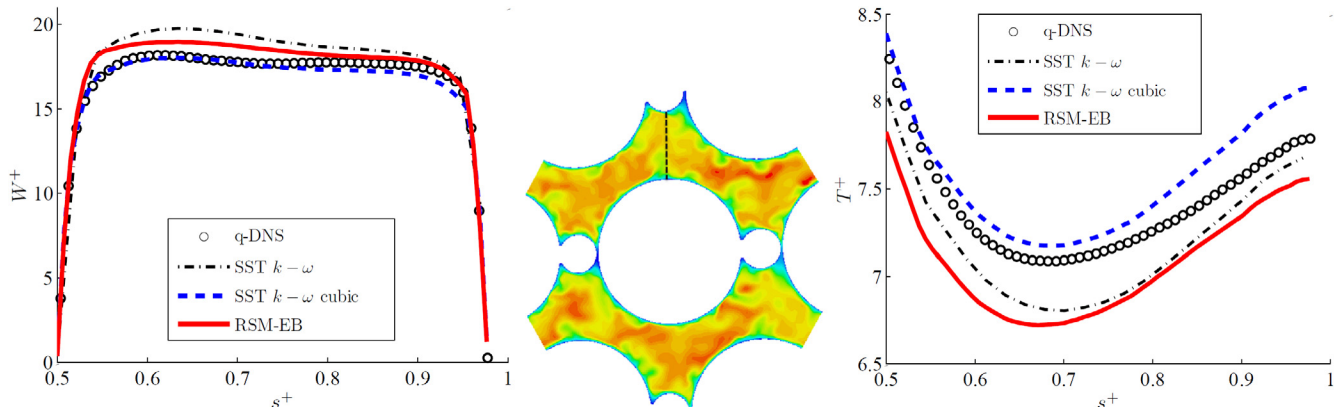


Fig. 12. Quasi-DNS instantaneous velocity field (middle) and comparison to various RANS models for mean axial velocity (left) and temperature (right) along the indicated line (middle).

**Table 1**  
Achieved accuracies for wire wrapped bundle simulations with RANS models.

Reference Data	Working fluid	Reynolds number	Turbulence models	Accuracy hydraulics (v/p)	Turbulent heat flux model	Accuracy heat transfer
7-pin LES	sodium	22,500–50,000	real. k- $\epsilon$ , SST k- $\omega$ , cubic k- $\epsilon$	10%	–	–
7-pin MIR	water	4000–15,000	SST k- $\omega$ , cubic SST k- $\omega$ , RSM-EB	t.b.d.	–	–
19-pin NACIE	LBE	1200–15,000	SST k- $\omega$	–	Pr <sub>t</sub> = 0.9	10%
19-pin KALLA	LBE	14,000–48,000	SST k- $\omega$	15% for pressure	Pr <sub>t</sub> = 0.9	12%
61-pin LES	sodium	19,000	SST k- $\omega$ , cubic SST k- $\omega$	5% for pressure	–	–
127-pin COMPLIT	LBE	4000–35,000	SST k- $\omega$	12% for pressure	–	–
Infinite pin (quasi DNS)	LBE	7000	SST k- $\omega$ , cubic SST k- $\omega$ , RSM-EB	10%	Pr <sub>t</sub> = 0.9 and 2	10%

result (middle).

## 7. Conclusions

The current paper describes a series of RANS validation efforts for wire-wrapped fuel assemblies ranging from small bundles (7 and 19 pins) to large bundles (61, 127 and an infinite number of pins). The accuracies achieved for all these simulations using RANS turbulence models are summarized in Table 1.

The accuracies achieved with the validation up to now indicate that an accuracy within 12.5% for engineering RANS models should be feasible for all bundle sizes and all parameters checked. Please note that this value has to be considered as preliminary. Important steps in the validation strategy are missing, i.e. validation for large scale bundles both for the hydraulic field as well as for the thermal field. Furthermore, it is important to realize that all of the applied thermal validation simulations have used the standard Reynolds analogy with a constant turbulent Prandtl number approach, while it is well known that application of more advanced turbulent heat transport models can improve the results as shown by Shams and De Santis (2019) for a number of increasingly complex test cases.

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