## Group: Framatome Professional School

# Annual report of the Framatome Professional School

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The Framatome Professional School (FPS) organizes training courses in safety technology, thermal hydraulics, reactor physics, stress analysis, and hydrogen technology etc. Courses are tailored for engineers specializing in new topics within Framatome and they are open for students from KIT and other universities. Moreover, through the regular exchange between KIT and Framatome public funding opportunities for joint proposals are identified.

The FPS coordinates the InnoEnergy Master Schools Programmme "Energy Technologies" which offers a broad-based education in a variety of key engineering disciplines. A focus lays on the inter-disciplinary aspects of the sustainable energy sector and an in-depth understanding of the role of innovation and entrepreneurship in the future energy industry. Students receive a Master's degree from two of the four participating universities (IST: Instituto Superior Técnico in Portugal, Grenoble INP: Institute of Technology in France, UU: Uppsala University in Sweden, or KIT). The FPS also organizes ex-curricular activities for students such as the annual SiemensEnergy New Energy Challenge.

The FPS has a long history of applied research and strong links to other ITES-groups exist. The FPS applies Computational Fluid Dynamics and System Codes, develops Reduced Order Models for Uncertainty Quantification and mesh-free modelling of three-dimensional thermohydraulic components, and exploits methods of applied mathematics such as asymptotic series expansions to complex physical problems.

The applied focus of the research of the FPS led to inventions in 2020. A lab-on-a-chip STOKES II developed by P. Marthaler and A.

Class allows driving  $\mu$ m-scale fluid flow on a chip in a freely programmable fashion. This provides a new platform technology for complex diagnostics and chemical synthesis tasks.

The FPS invention BattMarines addresses electric energy storage in a power-heat-power concept.

In the following sections a number of activities of the FPS are summarized.

# CFD Validation of heated rod bundles in heavy liquid metals

#### Abdalla Batta, Karsten Litfin, Andreas Class

In our group, validation of CFD models for thermal-hydraulic simulation is an essential part of our work. Recently many studies are performed for supporting the design of next generation reactors like the "Multi-purpose hybrid research reactor for high-tech applications (MYRRHA)" planned at SCK-CEN, Belgium. For this purpose a series of EU-projects have been started in the last years like EURO-TRANS (2005-2010), THINS (2010-2015), SEARCH (2011-2015) and MAXSIMA (2012-2018), to name a few.

The ongoing Project PATRICIA (2020-2024) aims to support safety studies for heavy liquid metal cooled fast reactor systems. The effect of a well-defined porous blockage in a wire spaced 19-pin rod bundle and the effect of rod bundle deformation will be experimentally investigated at KALLA with numerical support from our group. Further numerical support will given for the project PASCAL (2020-2024)



Figure 1: Schematic side view of a rod bundle test section in heavy liquid metal with two small blockage elements. All axial positions are expressed in mm, referring to the onset of the heated zone (z=0).

where the effect of deformation on the local flow and temperature field will be studied.

An example for the validation of experimental results obtained within the EU FP7 project "Methodology, Analysis and eXperiments for the Safety In MYRRHA Assessment (MAXSIMA) project will be presented in the following subsection. More details about the project can be found elsewhere [1], [2], [3]. Figure 1 shows the test section with two blockage elements (marked in yellow) installed at selected locations in the heated section (marked in red). Details of the study are given in [4].

## **Model validation**

In this example, we present a comparison of the experimental results to CFD calculations. To quantify the impact of the blockage (I) onto the local temperature we define the impact factor as:

$$I = 100 \frac{T_{blocked} - T_{unblocked}}{T_{blocked} - T_{inlet}}$$

The impact factor is presented for both the experimental and numerical data in Table 1. The evaluation employs temperature values measured behind the first blockage (Central one). From experimental data, one can see that wall temperature is influenced with maximum 10.9 % at the thermocouple  $T_{ML2_R16_240}$ , where the blockage impact on fluid reaches 22.7 % at  $T_{ML2_S41}$ . Considering the numerical results, it can be seen that the blockage impact is smaller than the experimental values and take place at different location. This shows that current models are not yet adequate to predict flow mixing around blockages.

For the comparison between numerical and experimental local results, the error (Err) can be calculated by:

$$Err = 100 rac{T_{experimental} - T_{numerical}}{T_{experimental} - T_{inlet}}$$

	Experimental			Numerical			Num. error comp. to Exp.	
type	temp. blocked	temp. Unblocked	I [%]	temp. blocked	temp. unblocked	I [%]	Err %	Err %
Case number	157	24		157	24		157	24
T_ML2_R1_270	278.31	278.64	-0.4	285.7	283.6	2.5	9.5	6.3
T_ML2_R6_330	276.64	276.56	0.1	281.6	281.0	0.7	6.4	5.8
T_ML2_R7_210	269.04	269.67	-0.9	274.7	278.7	-5.0	8.2	12.9
T_ML2_R16_240	257.11	251.51	10.9	246.9	243.1	8.7	-17.9	-16.2
T_ML2_R16_330	266.81	267.83	-1.5	264.1	268.5	-6.4	-4.1	0.9
T_ML2_R17_30	264.27	266.41	-3.2	269.4	271.7	-3.3	8.0	8.0
T_ML2_R18_150	263.95	266.2	-3.4	276.4	274.3	2.8	19.4	12.2
T_ML2_S5	262.83	260.75	3.4	274.4	266.3	12.3	18.5	9.1
T_ML2_S20	270.01	259.82	17.0	262.0	262.7	-1.1	-11.4	4.8
T_ML2_S21	261.59	257.19	7.7	262.0	258.9	5.2	0.7	3.0
T_ML2_S33	245.64	246.52	-1.9	259.3	249.9	18.9	30.0	7.3
T_ML2_S41	237.57	230.61	22.7	225.8	223.3	10.7	-31.2	-23.8

Table 1: Experimental and numerical temperature data for case 157 and 24 of the blocked rod bundle experiment at KALLA. All temperatures in [ $^{\circ}C$ ]

The calculated error values are given in the last two columns of the Table. Note that the maximum error is observed for the fluid temperatures measured near the outer wall. This can to some extent – be related to heat losses at the outer wall of the bundle which has been neglected in the simulation. However, the dominant reason is a weak capability of the model to predict turbulent liquid-metal flow with obstacles and strong circulation.

Based on the presented data the Nusselt number can be calculate yielding for the experimental data:  $Nu_{blocked} = 10.54$ and  $Nu_{unblocked} = 11.03$ . The value for  $Nu_{unblocked}$ is similar to the value Nu = 11.2 calculated based on comprehensive data. From the numerical data  $Nu_{blocked} = 9.73$ and  $Nu_{unblocked} = 9.88$  are obtained. Comparing experimental to numerical results for Nusselt numbers better agreement than for local temperatures is found. Thus, the blockage has a minor effect on the calculated Nusselt number, since the latter is based on the average temperature. Note that the predicted temperature error scatters exhibiting negative and positive values. Therefore, in the averaged values the

difference relative to simulated results is less when comparing local data to experimental data. Detailed discussion on the experimental results can be found in [5]

#### References

[1] Batta, A.; Class, A.; Pacio, J.; Numerical analysis of a LBE-cooled blocked 19-pin hexagonal wire wrapped rod bundle experiment carried out at KIT-KALLA within EC-FP7 project MAXSIMA" Paper ID 20532, Nureth 17, 2017.

[2] Pacio, J.; Daubner, M.; Fellmoser, F.; Litfin, K.; Wetzel, T.; Experimental study of heavy-liquid metal (LBE) flow and heat transfer along a hexagonal 19-rod bundle with wire spacers, Nuclear Engineering and Design, 301, pp. 111 – 127 (2016).

[3] Pacio, J., et.al.; Final report on partially blocked wire wrapped LBE rod bundle experiment, Technical Report, MAXSIMA Deliverable D3.4,2017. [4] Batta, A; Class, A.; Validation for CFD thermalhydraulic simulation for liquid metal cooled blocked 19-pin hexagonal wire wrapped rod bundle experiment carried out at KIT-KALLA, AMNT19, 2019.

[5] Pacio, J.; Daubner, M.; Fellmoser, F.; Litfin, K. und Wetzel, T.; Heat transfer experiment in a partially (internally) blocked 19-rod bundle with wire spacers cooled by LBE Nuclear Engineering and Design, 2018, 330, 225 – 240.

# Creation of a reduced order model for the k - $\epsilon$ model

#### Jorge Yanez, Andreas Class

#### Introduction

Nuclear technology is a sector in which safety is insured in a very strict manner. In these frames, is becomes crucial to analyze the statistical trustworthiness of Computational Fluid Dynamics (CFD) results. That is to assess the effect of the bias and the unavoidable random variation and aleatory disposition of the initial conditions of a realistic scenario. For this task Reduced Order Models (ROM) come to hand [3]. Here we address the creation of a ROM for the standard k- $\epsilon$ - turbulence model as it represents the "work horse" of CFD analysis. This is not a simple task since the k- $\epsilon$  model equations exhibit multiple non-linearities.

#### Theoretical model

We start with the formulation of the Navier-Stokes equation in its Boussinesq approximation and the complementary k- $\epsilon$  equations[4]. In our methodology [2], we utilize the Method of Snapshots [1] to create a simplified model. That is, we obtain the transient solution of our equations with the high fidelity solver STAR-CCM at times { $t_1, ..., t_n$ }. We form with them a snapshot matrix Y. We carry out its Singular Value Decomposition,  $Y = V\Sigma G^T$ . We project the *n* dimensional vectorial space in a-reduced-sub-space of dimension n - j dropping the last *j* vectors in *V*. The first n - j vectors of *V* create a vectorial space at most  $\sqrt{\sum_{i=j}^{n} \|\sigma_i\|^2}$  distant form the original one.

To develop the reduced order model, we write the k- $\epsilon$  equations in terms of the reduced order basis. We follow the same rationale as [3]. After a quite complex algebra, the model adopts the form,

$$\left(\mathbb{D} + \frac{\Delta t}{2} \mathbb{E} + \frac{\Delta t}{2} \mathbb{FJ}\right) \begin{pmatrix} \overline{\delta u} \\ \overline{\delta T} \\ \overline{\delta k} \\ \overline{\delta \epsilon} \end{pmatrix} - \Delta t \mathbb{G} = 0$$

Note that  $\mathbb{D}$ ,  $\mathbb{E}$ ,  $\mathbb{F}$ ,  $\mathbb{G}$  and  $\mathbb{J}$  are matrixes with a much smaller dimension compared to the degrees of freedom of the high fidelity calculation. They depend on the dimension of the reduced basis. Yet, the matrix entries depend on the comprehensive high-fidelity calculation. All matrix entries are calculated once during the post processing of the high-fidelity results, and subsequently stored.

#### Application

We apply our construct to a convection case of domain 10x10x1 meter and resolution 0.1 meter. We consider the volume completely isolated for the whole set of variables, with zero gradient perpendicular to the boundaries.

Considering the snapshots generated and a maximum distance of  $10^{-7}$  to the projection space, the dimensions of the reduced space is 25 considering all variables of the system. Note that that means that the--full--matrices of the model are in fact of size  $25 \times 25$  in total, compared with the dimension 100.000x100.000 of the—sparse--matrices of the original calculation for each variable.

The model has been implemented in an in house Python code. The results of the integration of the ROM compared with the original CFD results can be seen in Figure 2. The CFD result has been projected into the reduced basis. The amplitudes in this basis of the ROM and the CFD can be directly compared. We see an excellent agreement between CFD and ROM.



Figure 2 Comparing the reduced order model (ROM) with original CFD calculations show an excellent agreement. (top: velocity; bottom: k)

### **Conclusions**

We have shortly summarized the procedure we have followed for the creation of a reduced order model of the k- $\epsilon$  turbulence model based on Proper Orthogonal Decomposition and Galerkin projection. The model finally adopts a simple expression.

In the whole derivation procedure, on-line operations, that is, those to be done during the integration of the reduced model, have the complexity of the reduced basis. Only off-line operations, done once during the post processing the results of CFD have the complexity of the original basis. The construct obtained shows a very good performance reproducing the calculation proposed to illustrate its capabilities.

## **References**

[1] Berkooz, Gal; Holmes, Philip and Lumley, John L; 1993. "The Proper Orthogonal Decomposition in the Analysis of Turbulent Flows." Annual Review of Fluid Mechanics 25 (1): 539–75.

[2] Yáñez, Escanciano Jorge and Class, Andreas G.; 2019. "POD-Galerkin Modeling of a Heated Pool." Progress in Nuclear Energy 113: 196–205.

[3] Quarteroni, Alfio; Gianluigi Rozza, et al.; 2014. Reduced Order Methods for Modeling and Computational Reduction. Vol. 9. Springer.

[4] "STAR Ccm+ Users Manual." n.d.

# A free programmable lab-on-a-chip

Philipp Marthaler, Andreas Class

# Background

Lab-on-a-chip systems are utilized in many fields for rapid and reproducible chemical analyses on a microscale. Especially in medical technology, such tools support diagnoses and research. The design of most systems, however, is customized for one specific application. Important application cases are point-ofcare diagnostics or DNA sequencing. Such single-application systems are characterized by networks of micro-channels. Channel networks ranging from rudimentary (single-use systems) to complex (covering multiple use cases) are available.

In the described systems, probes are embedded and transported in a fluid environment. The carrier fluid which contains the diffuse samples is excited to flow by induced-charge electro-osmosis. Most common is the excitation with AC potentials applied via electrodes inside the channel wall. In contrast to the application of DC fields, that method has several advantages. In particular, it is applicable in more complex geometries and creates more continuous flow patterns.

#### Innovative approach

We developed a novel lab-on-a-chip system that does not depend on channel networks. The carrier fluid with diffuse probes is transported using AC electro-osmosis with traveling waves, also known as traveling wave electroosmosis.

The central element of the development of that system is a spectral code that simulates the underlying electro-hydrodynamic phenomena. With that code, an earlier ITES patent [1] was examined for its effectiveness and feasibility. Based on the results, the excitation method was improved from alternating current to traveling waves. The code was further utilized to find the optimal operating parameters for the system based on fluid properties, ion species, and concentration. Compared to most available systems, high transport velocities were reached.

The optimized excitation method can now be applied in a redesigned 1mm x 1mm chip (schematically shown in Figure 3) with a free flooded surface. Channels are not necessary for this system. Thus, many processes can be performed on one chip. Those processes depend mainly on the software implementation and only to a minor part on the chip geometry.



Figure 3 Schematic sketch of the chip structure. Dark blue paths represent example flow patterns in the flooded surface (light blue). The electrodes are controlled by single control units (black squares) and are responsible for flow excitation.

Besides flow excitation and probe transport, the design of a wire network inside the chip supplying a large number of electrodes was an immense challenge. For the prototype design and numerical verification, Philipp Marthaler and Andreas Class won the 2nd prize at the KIT innovation contest NEULAND [2]. The award ceremony is shown in Figure 4.



Figure 4 Award ceremony of the NEULAND contest.

#### **References**

[1] Class, Andreas; Barz, Dominik; (2006): Arrangement for generating liquid flows and/or particle flows, method for producing and operating said arrangement and use of the latter, (WO 2007/090531 A1), World Intellectual Property Organization

[2] Marthaler, Philipp; Simon, Marie; (2020): Interview with the nominees of the NEULAND Innovation Contest, KIT Research to Business Online Portal (https://www.kittechnology.de/en/blog/interview-nominees-ofthe-neuland-innovation-contest, 26.04.2021, 16:10) the concept appears to be naïve, it offers remarkable advantages with respect to its scalability to the anticipated large storage capacity. The steam within the thin-shell storage vessel is stored at the ambient pressure of the surrounding water at large depth and thus exhibits high energy density. The heat losses of the storage vessel and the steam line are obviously quiet large but in comparison to the huge energy contents, they become acceptable, so that storage times ranging from several hours to seasonal storage become feasible.



**BattMarines** 

Abdalla Batta, Andrea Bellelli, Karsten Litfin, Andreas Class

A mayor challenge of the Energiewende is energy storage to bridge periods where neither wind nor photovoltaics can provide renewable energy sources. For the success of storage solutions in the market, both a low price and an acceptable efficiency are equally relevant factors. Power-Heat-Power solutions for energy storage accept compromises with respect to the achievable efficiency and aim at low system prices to become competitive. The novelty of the proposed BattMarines is to use a conventional Rankine-cycle in batch operation as an energy storage system and to exploit scaling to large dimensions (storage capacity ~1 GWd) to reach economical goals.

Figure 5 shows a schematic sketch of BattMarines [1]. A high-efficiency steam turbine power plant is installed on a floating platform on the sea. A huge tank resides on the seabed and contains large quantities of hot live steam. To produce electric power on demand steam is drawn through the vertical steam line connecting the platform and the storage vessel. Charging the system is accomplished by electrically heating fresh water when a surplus of renewable energy becomes available. Even though

Figure 5 Sketch of BattMarines Power-Heat-Power storage concept.

#### **References**

[1] Class, A. (2020); BattMarines, 2<sup>nd</sup> International Workshop on Carnot Batteries 2020, University Stuttgart, September 15.-16, 2020.