CFD SIMULATION OF ROD BUNDLES K. Podila, J. Bailey, Y.F. Rao, and M. Krause

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Abstract

Atomic Energy of Canada (AECL) has initiated a program to develop Computational Fluid Dynamics capability (CFD) to simulate single-phase and two-phase flow conditions in rod bundles. This paper presents a comparative analysis of turbulence models available in commercial CFD programs for their use in nuclear thermalhydraulic applications. The objective was accomplished using ANSYS FLUENT 6.3.26 for two geometries: a 5×5 bundle with split-type spacers and a 28-element bundle with appendages. Apart from the analysis of the two- and seven-equation models, superior predictive capabilities of the DES (Detached Eddy Simulation) and LES (Large Eddy Simulations) approaches were demonstrated for the 28-element uncrept CANDU fuel channel with appendages.

1. INTRODUCTION

Accurate prediction of the flow and heat transfer in fuel bundles is important in design and safety analysis of nuclear reactor systems. Turbulent mixing is a significant phenomenon that strongly affects the flow and enthalpy distribution in subchannels of a fuel bundle, which in turn affects the thermalhydraulic performance of the bundle. This is especially true for bundles with small pitch-to-diameter ratio (P/D) [1]. Even for bare bundles, i.e., bundles without appendages such as spacers and endplates, modelling of turbulent flows remains a challenge due to the presence of large-scale unsteady coherent turbulence structures (flow pulsations) and turbulence-driven secondary flows.

Despite the advancements made in turbulence modelling and numerical simulation, the CFD approach fails to accurately predict distributions of velocity, temperature, wall shear stresses and turbulent mixing when the P/D ratio is smaller than a threshold value [1]. In most of the previous investigations of tightly-packed rod bundles [2], the RANS (Reynolds Averaged Navier Stokes) models were employed although their limitations were well documented.

In rod bundles, the complexity of the geometry and non-uniformity of the flow introduces secondary flow structures that can only be captured with an unsteady three-dimensional CFD approach. Further, the turbulent mixing around a narrow gap is largely determined by the anisotropy of turbulence structure in the region, which cannot be resolved with the RANS approach. Therefore, in order to simulate these secondary flows, either the URANS (Unsteady RANS) approach with a turbulence model that provides each component of Reynolds Stresses, or an advanced formulation such as DES or LES should be used ([3] and [4]). Recently, guidelines developed at university of Ottawa [4] recommend URANS for flows in tightly packed rod bundles with P/D<1.2.

The overall objective of the research project is to develop the capability of CFD to accurately predict the fluid flow and heat transfer in fuel channels. The focus of the current investigation is to provide comparative analysis of turbulence models for single-phase flows which forms Phase I of the project. From a CFD point of view, the ability to accurately predict velocity and turbulent secondary flow structures is important, even before attempting to predict two-phase flows and CHF (Critical Heat

Flux). Once the methodology for successfully predicting single phase flows is accomplished, Phase II of the project will focus on developing a two-phase flow capability for rod-bundle flows.

The ability of CFD to capture the flow physics of rod bundles will be assessed by comparing the predictions with experiments. AECL is participating in a blind benchmark organized by the OECD/NEA for the MATiS-H¹ facility [5] to gain direct access to the reliable experimental data, tentatively planned to be released by organizers in May 2012. The description of MATiS-H experimental setup and summary of Canadian participation in the CFD benchmark is discussed in [6].

In this current investigation, the ability of turbulence models to predict the secondary flow structures is tested by simulating experiments on a cold 5×5 bundle with split-type spacers. Also, a detailed assessment of the turbulence model under industrially relevant conditions was made by comparing simulations against experiments on a string of 28-element bundles in an uncrept CANDU² channel performed at Stern Labs (SL) [7].

2. COMPUTATIONAL MODEL

The simulations for the 28-elements uncrept CANDU channel were performed on a local workstation, AECL CU12³. Due to higher computational requirements for the 5×5 rod bundle with split-type spacers, AECL CU199⁴ was used. In order to reduce the computational run time, a parallel version of ANSYS FLUENT 6.3.26, capable of executing on eight nodes was used.

2.1 Development of Simulation Domain

In the current investigation, GAMBIT 2.4 was used to develop mesh for the 28-element uncrept CANDU fuel channel with appendages (Figure 1). The attempts of meshing the 5×5 bundle with split-type spacers using GAMBIT was found to be time consuming and led to highly skewed meshes. Hence, ANSYS meshing software was utilized for meshing the 5×5 rod bundle with split-type spacers. Because the split vanes induce swirl in the flow, no symmetry planes were used, as the use of this boundary condition would force a symmetric condition even if this was not the correct solution.

On the other hand, to reduce run times, for a 28-element uncrept CANDU channel (Figure 2), a symmetry boundary condition was imposed along the vertical axis of the channel and only half of the fuel channel was modelled in the current problem. Although, using full computational domain would lead to higher accuracy but this would in turn result in exceedingly high solution run times. Since the geometry of the endplates and the 28-element fuel bundles was different, the two domains were connected using a non-conformal interface.

In order to make a quick analysis, a standard wall function with dimensionless wall distance $(y^+)\sim 30$ was used which is generally considered as the rule of thumb for the placement of first node point in the domain. Geometry decomposition was done in areas where meshing was expected to be particularly challenging. The use of tetrahedral cells was avoided in the current investigation except for 5×5 bundles with the split-type spacers, for which a hybrid mesh (hexahedral+tetrahedral+prism cells) was used.

¹ MATiS-H (Measurements and Analysis of Turbulence in Subchannels-Horizontal) is a test facility located at Korean Atomic Energy Institute (KAERI), used to perform experiments on 5×5 bundle with split- and swirl-type spacers.

² CANDU (CANada Deuterium Uranium) is a registered trademark of Atomic Energy of Canada Limited (AECL).

³ AECL CU12 is a 32-bit, dual core AMD Opteron processor-880 operating on Linux with 32 Gb of RAM.

⁴ AECL CU199 is a 64-bit, Hex core HP Z 800 workstation with 64 Gb of RAM and 1 TB hard drive.

For all the current assessment, predicting near wall characteristics was of prime importance. Hence, it was ensured that at least four cells in the boundary layer were applied to the wall surface (Figure 3). Due to the total mesh size being close to the hardware limit of 11-15 million elements, boundary layers were not used for the 5×5 bundle as this would have put the mesh size well over the limit (Figure 4). In order to maintain a relatively low cell count, coarse meshes were used along the length of the domain and fine meshes (at least seven cells) were used between rod-to-rod gaps. For the two geometries tested, the individual mesh count varied from 12 million cells up to 15 million cells.

For all the rod-bundle configurations, the entrance and exit of the flow channel were simulated by using a uniform mass-inlet and pressure-outlet boundary condition. The fuel rods, the attached spacers and the bearing pads were set as solid walls with no-slip conditions. For the heated test cases, the surfaces of the rods were set to a constant heat flux condition whose value was set to match the experimental axial and radial heat flux distributions.

2.2 Solution Methodology

The fundamental flow, energy, turbulence kinetic energy and dissipation equations for a single-phase problem were solved using a 3-D double precision solver. The effect of gravity was included for completeness of the computational model even though its effect is negligible and thus commonly neglected. The solver selected for this study was a segregated solver based on the point Gauss-Seidel technique with multigrid V-cycle acceleration.

For both DES and LES runs, default numerical settings as specified in [8] were used. The default under relaxation factors (URF's) were used except for momentum and energy which were reduced to 0.5 and 0.99 respectively for all the URANS runs. The tightening of the URF for momentum and energy was primarily done to improve solution convergence and prevent excessive jumps in residuals which lead to numerical divergence.

On the other hand, DES and LES use tighter URF's of 0.5 for all the parameters in order for the solution to proceed smoothly. The viscous, pressure and convective terms were discretized using first order schemes. Pressure-velocity coupling was achieved using a SIMPLE algorithm. For all the URANS runs, a time step size of 0.01 s and four iterations per time step within a single iteration was used. The temporal discretization in the current investigation was achieved using first-order implicit time differencing scheme built in ANSYS Fluent.

Iso-surfaces were created near the inlet, centre and exit of the channel to monitor the variation of velocity and temperature to judge the solution convergence. The solution was considered to be converged at that particular surface once the monitored parameter leveled off to a certain value and did not change by more than 0.02% for the next 300 iterations. Since the Reynolds Stress Model (RSM) requires more computational effort and leads to more difficulties with convergence than the k- ϵ model, a convergence strategy was utilized in the present work in which the k- ϵ model was used as a starting point for the RSM [8]. This helped eliminate the crude initial guesses for k and ϵ and prevent solution divergence. Similarly, an instantaneous velocity field for LES was generated using fully converged RANS. The conversion was achieved using a synthetic turbulence generation routine in ANSYS Fluent. This served as a starting point for the case of LES simulations, which helped to accelerate convergence and reduce run times.

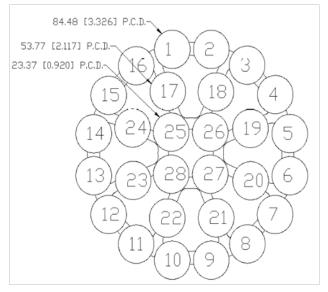


Figure 1 Cross-Sectional Geometry of the 28-Element CANDU Bundle (Not Including Appendages) and the Element Identification Scheme (from [7])

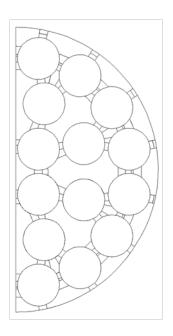


Figure 2 Cross-Sectional Geometry used in Mesh Generation for the 28-Element Fuel String Simulation



Figure 3 2-D Cross-Section of a Hexahedral Mesh used in the Present CFD

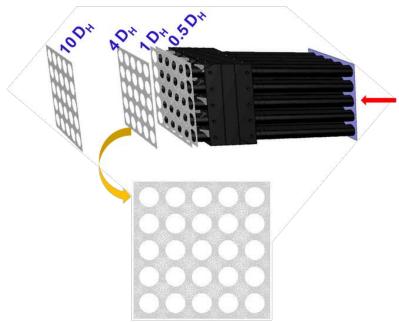


Figure 4 Solution Domain and 2-D Cross-Section of Hybrid Mesh Used in CFD Simulation of 5×5 Bundle with Split-Type Spacers

3. RESULTS AND DISCUSSION

3.1 Comparative Analysis of Turbulence Models for the 5×5 Rod Bundle with Split-Type Spacers

In the present study, two turbulence models, the standard k- ϵ model and the RSM using linear pressure-strain model were tested. The model constants present in the k- ϵ and RSM were not modified in the current investigation. The widely used k- ϵ model was tested though it assumes isotropy of turbulence where normal stresses are equal. On the other hand, the RSM accounts for anisotropy in the stresses resulting in prediction of secondary flows.

As can be seen from Figure 5, both k- ϵ model and RSM predicted comparable relative turbulence intensities defined as:

$$\sqrt{0.66 \times k} / V_{magnituds}$$
 (1)

where, k is the turbulence kinetic energy. However, the k- ϵ model uses Boussinesq's hypotheses and cannot correctly predict the velocity fluctuations in the three components. Hence, RSM turbulence model was used for modelling of 5×5 rod bundles with split-type spacers.

As can be seen from Figure 6, the turbulence intensity was observed to be highest at 0.5 hydraulic diameter (D_H) downstream of the split-type spacers. As expected, the effects of the mixing vanes on turbulence intensity are gradually weakened after the 1 D_H from the spacers grid (Figure 6).

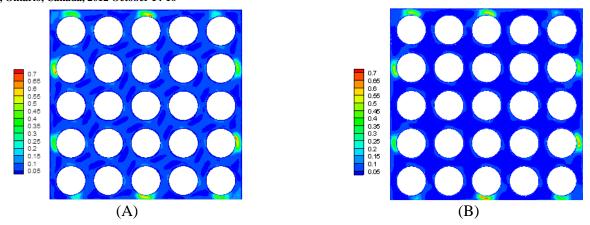


Figure 5 Effect of Turbulence Models on Relative Turbulence Intensity Predictions for 5×5 Bundle with Split-Type Spacers at 0.5 D_H Downstream of Spacers (A) URANS k-ε; (B) URANS RSM; (P/D =1.30, Mass flow=24.2 kg/s)

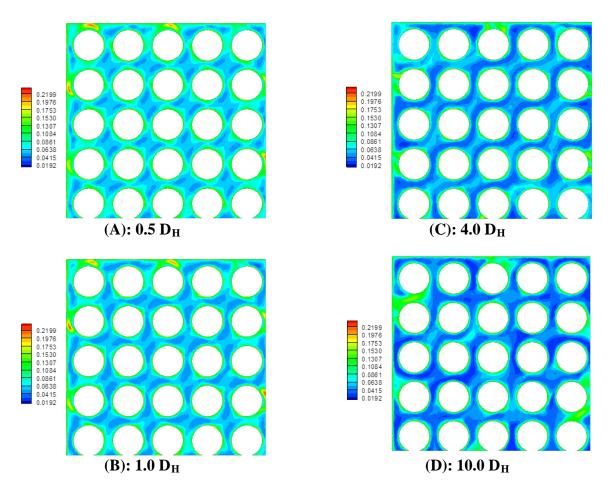
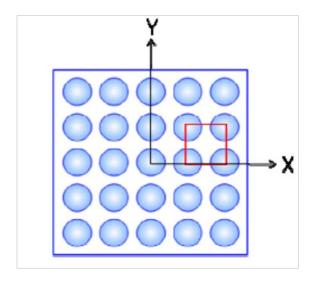


Figure 6 Turbulence Intensity (\sqrt{ww}) in the Axial Flow Direction (z-) Downstream of Split-Type Spacers Using URANS RSM (P/D=1.30, Mass Flow=24.2 kg/s)

The circulation was calculated downstream of the spacers at the specified subchannel in the four cross-planes downstream of the spacer-grid exit plane. The circulation (Γ) in the specified subchannel (Figure 7) is estimated using Equation (2), where ω_z is the z-component vorticity.

$$\Gamma = \iint \omega_z dxdy$$
 (2)

In contrast to some previous investigations (e.g., [9] and [10]), which neglected the gap regions for estimation of the subchannel vortex circulation, the complete subchannel area was used for calculation in the current investigation. The current solution methodology predicted circulation in the clock-wise direction which gradually decayed downstream of the spacer (Figure 8).



0.018
0.016
0.014
0.012
0.012
0.008
0.008
0.006
0 50 100 150 200 25C

Position, (mm)

Figure 7 The Subchannel Marked for Calculating the Flow Circulation (from [5])

Figure 8 Variation of Circulation at Four Cross-Planes Downstream of the Spacer-Grid Exit Plane

3.2 Comparative Analysis of Turbulence Models and Model Assessment Using 28-Element Uncrept CANDU Fuel Channel with Appendages

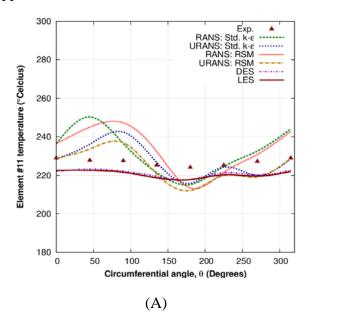
The 28-element CANDU fuel channel was simulated using 11 million cells with RANS and URANS. The model assessment was performed by comparing predictions with the experimental results from SL at Bundle #11 of the fuel channel. Significant differences in temperature predictions were seen (Figure 9) for the turbulence models tested. The RANS approach was also tested for its ability to capture the flow physics of the rod bundles. The RANS although quick (approximately two days for k-ε model varied up to three days for RSM) compared to URANS, cannot account for the unsteady flow pulsations in rod-bundles. As can be seen in Figure 9, RANS always predicted higher temperature variations compared to URANS results, irrespective of the turbulence model used. This is because of its inability to correctly account for turbulent flow pulsations.

Using the results from the steady state solution, the average run time for URANS simulations was approximately five days. Further, both models resulted in a non-uniform temperature variation along the circumference of the elements. According to the comparison with experiments, the RANS k- ϵ model predicted the highest temperature variation whereas; URANS RSM resulted in the least temperature variation. However, the simulated results using URANS RSM over-predicted the experimental measurements.

Anisotropic turbulence models such as the RSM are successful to a limited extent but they are incapable of predicting correct quantitative results for temperature distribution. This occurs due to the

inability of the current models to account for the flow pulsations phenomena as well as the presence of the secondary flows in the gap region. This limitation of the models (*k*- ϵ , RSM) suggests the need for exploring other advanced turbulence modelling approaches such as DES and LES. In order to resolve the unsteady flow behaviour these approaches demand much finer meshes and smaller time steps. However, in order to perform a scoping study to assess the ability of the models to correctly predict for mixing in rod bundles, a coarse mesh of eleven million cells was used for both DES and LES. The LES typically took more than two weeks to converge whereas for the same mesh, DES converged within nine days.

As can be seen from Figure 9, the use of DES and LES simulations resulted in a uniform temperature distribution profile compared to the RSM. Both DES and LES predicted similar results for the element #11 with slight under prediction of eight degrees. On the other hand, a good agreement was achieved for element #16 using LES. These comparisons performed on coarse mesh show the potential of DES and LES approach to accurately predict the turbulence mixing phenomenon and produce results that are closer to the experimental values. However, URANS with the RSM is much more cost effective in terms of the computational run times and hence is recommended for rod-bundle applications.



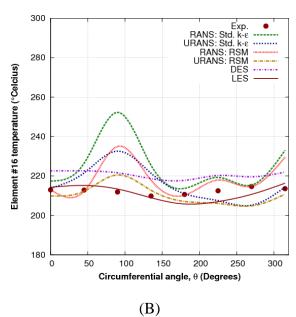


Figure 9 Effect of Turbulence Models on Circumferential Temperature Distribution at Bundle #11 for; (A) Element #11; (B) Element #16 (Mass-Flow Rate=13.51 kg/s, Operating Power=2,000 kW, Inlet Temperature=180°C)

4. CONCLUSIONS

The focus of the current study was to perform a comparative analysis of turbulence models using CFD for simulating rod bundles. Based on simulation results of two geometries, including a 5×5 bundle with split-type spacers and a 28-element bundle with appendages, the following conclusions can be made:

• Steady RANS simulation approach, though computationally faster than URANS should not be used for modelling CANDU bundles since it cannot account for the unsteady flow pulsations phenomenon.

- The RSM is better suited than k- ϵ for rod-bundle applications since it can account for the anisotropy in turbulence and thus has the potential to predict secondary-flow structures.
- For the 28-element uncrept CANDU fuel channel, the quantitative agreement is poor between predicted and measured wall temperatures. RANS *k*-ε predicted the maximum temperature variation whereas URANS RSM predicted the least.
- LES, even with a coarse mesh, resulted in closer agreement with the SL experiments. However, in order to resolve the large eddy present in the solution domain, a mesh much finer than the present one would be required.
- URANS RSM is recommended for modelling CANDU bundles since it accounts for turbulence anisotropy and is much more cost effective than LES.

5. ACKNOWLEDGEMENTS

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