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Potential of Serpent-OpenFOAM Coupled Codes for Spent Nuclear Fuel Analysis

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ABSTRACT

Operation of future district heating source Teplator with spent nuclear fuel assemblies requires deep analyses. The present article focus on a potential use of coupled neutronics and thermal-hydraulics codes for simulations with the spent fuel. The simulations were conducted in the neutronics code Serpent and the open-source CFD package OpenFOAM. Both codes were externally coupled operating at a prescribed number of loops. The goal of the study was to evaluate the influence of thermal-hydraulics (TH) feedback in investigation of the spent nuclear fuel. First coupling tests were conducted on a fuel pin of the VVER-440 fuel assembly. Results obtained from the coupled simulations showed a relatively small difference in the predicted heat power distribution between simulations with and without TH from OpenFOAM. Further, the greatest relative difference in coupled loops was between first two coupling loops with overall difference less than 3 % and the difference at the third loop was less than 0.1 %.

1 INTRODUCTION

A future district heating source Teplator [1] enables an operation with spent nuclear fuels. A reactor operation with spent nuclear fuels requires detailed safety analysis using thermal-hydraulics and neutronics calculations. Nowadays, the computational performance enables three dimensional thermal-hydraulics calculations of a reactor core and fuel assemblies using CFD software for various scenarios [2, 3, 4]. Widely used open-source CFD software OpenFOAM [6] serves well as a base for more complex solvers [5] and the neutronics code Serpent [7] reads an unstructured computational grid directly in OpenFOAM format [8] which favorites their use for coupled calculations. Coupled OpenFOAM-Serpent simulations were recently conducted for steady state, fuel burnup analyses [8, 9] and thermal-mechanics simulations [10].

The present work address modifications of OpenFOAM for coupled thermal-hydraulics and neutronics simulations with a spent nuclear fuel and further analyses a relative difference between coupled loops.

2 NEUTRONICS

Neuctronics calculations were performed using Serpent (Serpent 2.1.32) [7] and ENDF/B-VIII.0 continuous energy nuclear data library [11]. The geometry of the fuel pin was generated in Serpent and the multi-physics interface was used to read OpenFOAM mesh (Fig. 1 left). The fuel materials were distributed into 42 axial layers and the distribution is shown in Fig. 1 on right. The materials and burn-up were generated in WIMS/Moby-Dick.

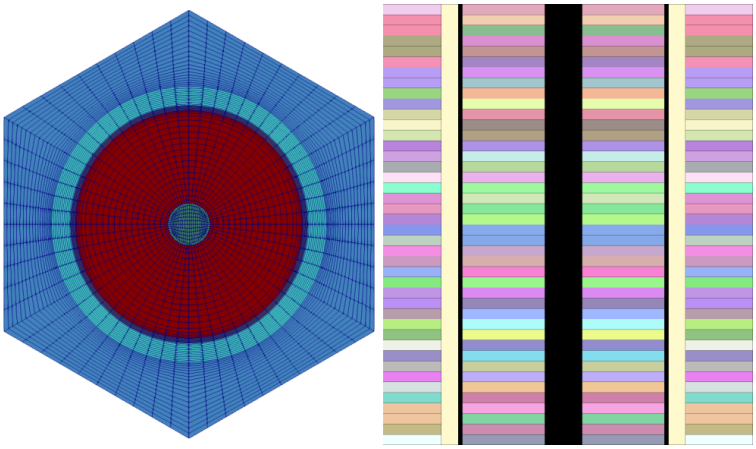

Figure 1: Computational grid and geometry of the fuel pin with axially distributed fuel materials.

Neutronics simulation consists 50 000 neutron population and 60 inactive and 560 active cycles. Thermal power of the fuel rod was set to 10 kW. Reflective boundary was applied at the radial borders of the domain and vaccum at the axial borders of the domain.

3 THERMAL-HYDRAULICS AND TURBULENCE MODELLING

The averaged continuity, momentum and energy equations of steady state flow

$$\nabla \cdot \overline{\rho}\overline{U} = 0, \tag{1}$$

$$\nabla \cdot \overline{\rho}\overline{U}\,\overline{U} = \nabla\overline{p} + \nabla \cdot \overline{\tau} + \nabla \cdot \tau_{turb} + S_M, \tag{2}$$

$$\nabla \cdot \overline{\rho}\overline{U}\,\overline{h} = -\nabla \cdot \overline{q} - \nabla \cdot q_{turb} + S_H \tag{3}$$

where $\overline{h}$ is the enthalpy, $\overline{p}$ is the pressure, $\overline{q}$ is the heat flux, q_{turb} is the turbulent heat flux, S_H is the heat source, S_M is the momentum source, $\overline{U}$ is the velocity, τ is the shear stress tensor, τ_{turb} is the second order tensor of Reynolds stresses.

3.1 Turbulence modeling

In order to close averaged governing equations, two linear RANS turbulence models based on the Boussinesq's approximation were used in the present study, namely k-ω SST [12] and k-ω TNT [13] models. Both models are widely used for calculations of iso-thermal and non-isothermal flow in engineering applications, however they struggle with a correct prediction of unsteady heat transfer such as heat transfer in separating and reattachment flows. To overcome this issue, Scale-Resolving-Simulations (SRS) models are nowadays used for unsteady simulations of heat transfer [14, 15]. The SRS models are planned to be evaluated after first steady-state tests.

The turbulent thermal diffusivity close to a wall was calculated using the Jayatilleke wall function.

$$\Theta^* = \sigma_t \left(U^* + P^* \right) \tag{4}$$

where the dimensionless velocity and Jayatilleke P-function is calculated as

$$U^* = \frac{1}{\kappa^*} \ln \left(E y^* \right) \tag{5}$$

$$P = 9.24 \left[\left(\frac{\sigma}{\sigma_t} \right)^{3/4} - \left(\frac{\sigma}{\sigma_t} \right)^{1/4} \right] \tag{6}$$

and normalization was as

$$U^* = \rho U k_r^{1/2} / \tau, \, , \Theta^* = \left(\Theta_w - \Theta \right) \rho C_p k_r^{1/2} / \dot{q}_w'', \, y^* = \rho y k_r^{1/2} / \mu \tag{7}$$

$$P^* = c_\mu^{-1/4} P, \, \kappa^* = c_\mu^{-1/4} \kappa, \, E^* = c_\mu^{-1/4} E \tag{8}$$

3.2 Computational settings

The flow was calculated as a steady state using the SIMPLE algorithm with 2 additional non-orthogonal corrector steps. Second order upwind discretisation scheme was used for divergence terms, Gauss linear for Laplacian terms and Least-squares for gradients. The convergence criterion for enthalpies and pressure was 10^{-8} and for velocities and turbulent properties was 10^{-6}. Flow parameters used in the present study are summarized in Table 1.

Table 1: Flow parameters

Inlet velocity	3.2 m/s
Inlet temperature	541 K
Reference pressure	12.2 MPa
Turbulent intensity	5 %
Viscosity ratio ν_t/ν	100
Pin power	10 kW

Thermophysical properties of water were calculated based on a polynomial fit of the IAPWS-IF97 data. An implementation of IAPWS-IF97 calculations into the OpenFOAM is currently under development and will be validated in a future work. Thermal conductivity and specific heat capacity of UO_2 and cladding were calculated based on MATPRO [16].

Spacer grids were simplified using a porous media approach [17] and the pressure drop was calculated as

$$\Delta p = 0.5 C_v \varepsilon^2 \rho U^2 \tag{9}$$

where the blockage ratio calculated as

$$\varepsilon = \frac{A_{gridspacer}}{A_{flow}} \tag{10}$$

and the drag coefficient C_v

$$C_v = 3.5 + \frac{73.14}{Re^{0.264}} + \frac{2.79 \cdot 10^{10}}{Re^{2.79}} \tag{11}$$

As full core simulations would require enormous computational performance, a coarse-mesh methodology [18, 19, 3] and local grid refinements methods [20] will be used in future calculations in order to decrease computational cost of coupled simulations.

3.3 OpenFOAM modifications

Numerical analyses of a nuclear reactor operating with a spent nuclear fuel using the coupled OpenFOAM-Serpent codes requires several additional libraries and packages in OpenFOAM solver. The first addition was an utility for the distribution of various fuel materials within one region. The utility used cell zone distribution and created a dict in the format required by Serpent. Further, the conjugate heat transfer solver *chtMultiRegionSimpleFoam* was modified in order to read the volumetric heat source from Serpent and to correctly calculate fluid-solid interface [8].

Calculations of thermophysical properties of fuel and cladding were implemented via new classes and the implementation of IAPWS-IF97 is under development.

3.4 Coupling script

The process of coupling with solver preparations was automated using a main Bash script. Workflow of the script is shown in Fig. 2. The first operation of the main script is an input preparation. The preparation is done by a Python script which reads the Serpent input file and creates several *topoSetDict* files (used by *topoSet* application to create the region cell zones for a mesh split operation and for Serpent material definition) and *setFieldsDict* files (used by *setFields* to initialise temperatures of coolant, cladding and fuel. The second part of the main script is a solver preparation where cell zone regions are created, boundary conditions are set and fields are initialised. The last part of the main script is the coupling loop. The coupling of thermal-hydraulic and neutronics is currently written to operate with a prescribed number of loops and the algorithm only check residual convergence. Due the external coupling, each loop contains mesh decomposition and reconstruction in order to read output values.

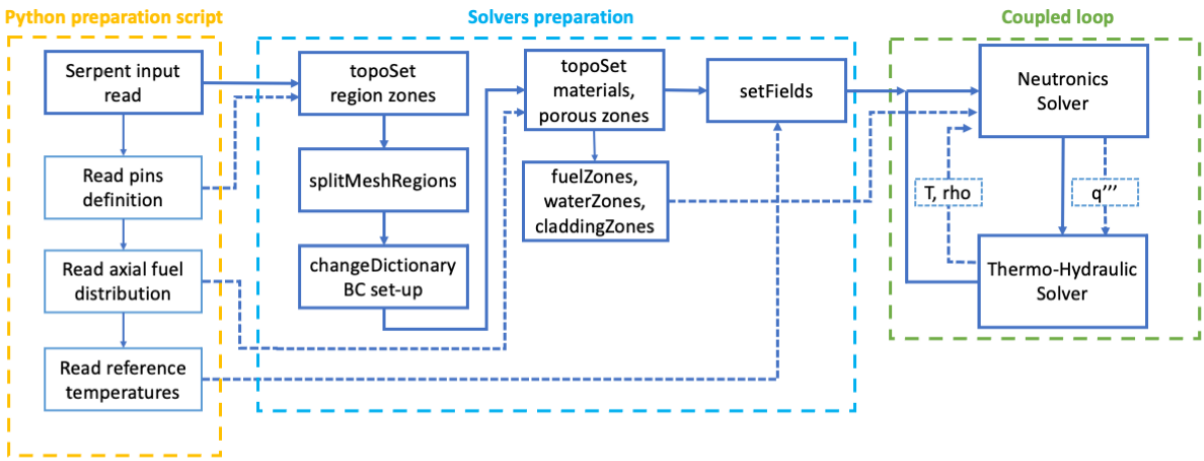

Figure 2: Coupling script scheme.

4 RESULTS

4.1 Fuel pin simulations

First tests of the coupling were conducted on one fuel pin. Comparison of predicted axial distribution of liner heat power with and without thermal-hydraulic feedback obtained from OpenFOAM is shown in Fig. 3 left and the corresponding relative error in Fig. 3 right. The

highest difference is in the upper part of the pin. The overall difference in the distribution is less than 1.5 %.

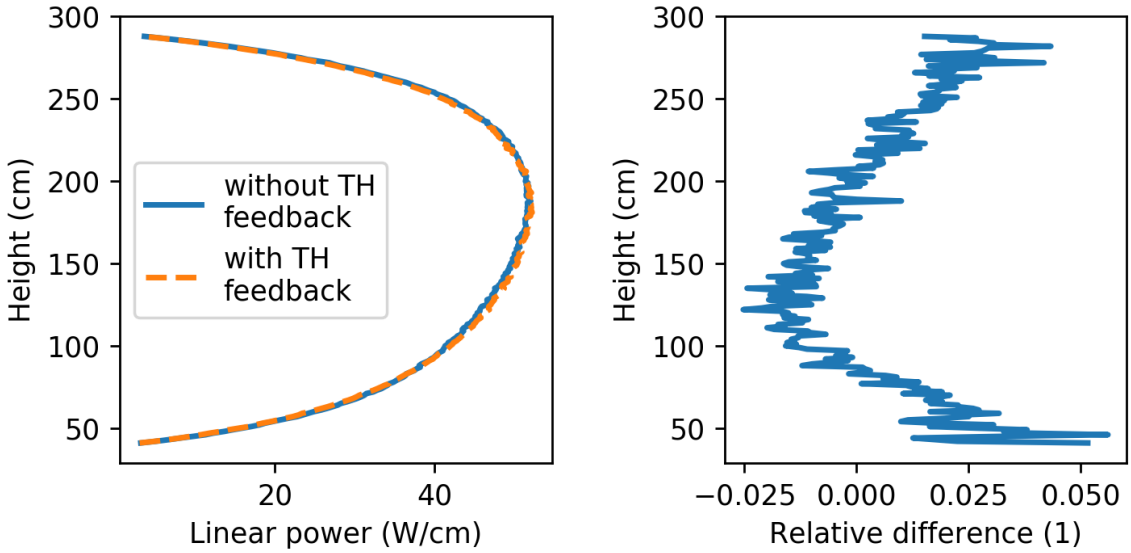

Figure 3: Axial distributions of liner heat power.

Several coupling loops were simulated in the present study and the highest difference was between first and second iteration loop. After the second loop the difference was less than 1 %. Comparison of axial profiles of the fuel surface temperature from the first and second iterations and corresponding relative difference are shown in Fig. 4.

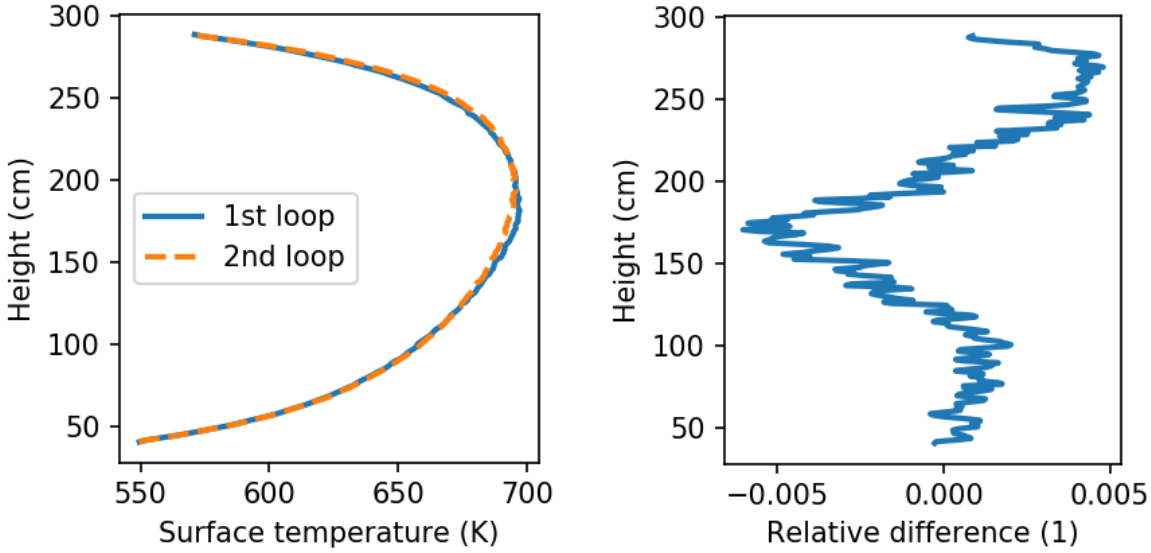

Figure 4: Axial distributions of fuel surface temperature.

Comparison of temperature profiles obtained by k-ω SST and k-ω TNT turbulence models is shown in Fig. 5. Both models predicted similar temperature profiles. The highest difference in the predicted temperature was close to the wall, however the difference is negligible as is lower than 0.2 %. Additionally, the simulation on a coarser grid predicted temperature profile

with a maximum relative difference 0.5 %. The averaged y^+ was 5 and the maximum value was lower than 10.

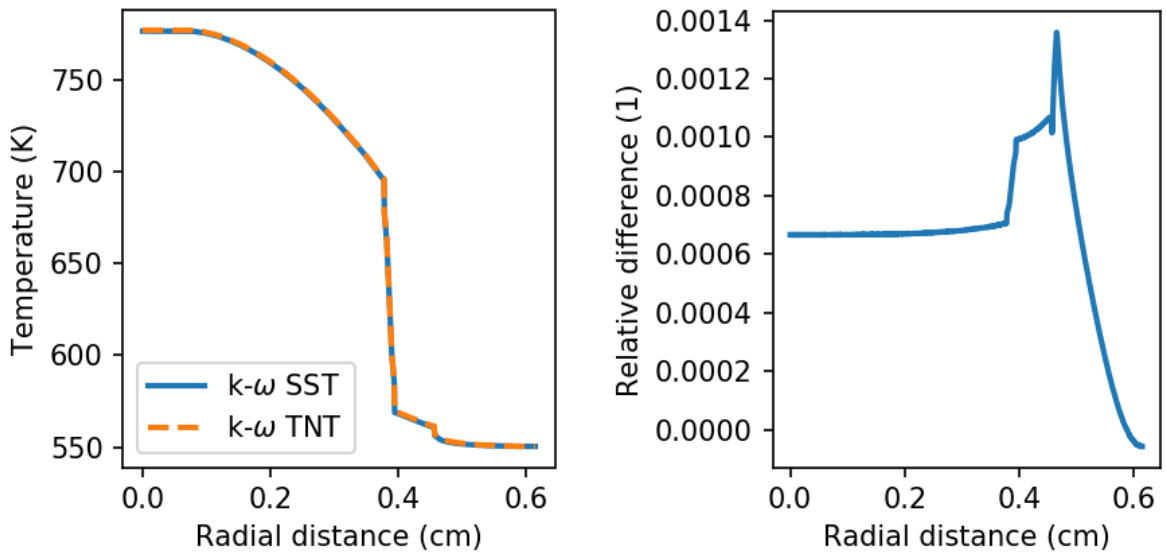

Figure 5: Radial distributions of temperature at height 164 cm.

5 CONCLUSION

The present study investigated a potential use of coupled OpenFOAM and Serpent codes to study a nuclear reactor operating with a spent nuclear fuel. Conducted simulations provided a closer insight into the temperature distribution in the fuel, cladding and coolant region and results will serve in future studies where operation conditions of Teplator reactor will be simulated. The present study compared predicted linear heat power with and without thermal-hydraulics feedback obtained from OpenFOAM where the overall difference was lower than 1.5 %. Further, the influence of turbulent model on predicted temperature profiles was negligible.

In future, the study will be extended for unsteady simulations on one fuel pin along with simulations on a simplified fuel assembly.

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