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OpenFOAM Analysis of CANDU-6 Moderator Flow

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1. Introduction

The horizontal fuel channels in a CANDU-6 reactor (a pressurized heavy water reactor) are submerged in the heavy water (D_2O) pool which is contained by a cylindrical tank, calandria. Each fuel channel consists of concentric tubes: a Pressure Tube (PT) and a Calandria Tube (CT). And the CO_2 gas is filled between these tubes. One of the important design features of the CANDU-6 reactor is the use of moderator as a heat sink during some postulated accidents such as a large break Loss Of Coolant Accident (LOCA). If the PT is sufficiently hot while the channel pressure is still relatively high, the PT may radially deform and would fully contact with its surrounding CT (PT/CT ballooning contact) as shown in Fig. 1.

Consequently, a heat flux is rapidly transferred to the outer CT so that a film boiling may occur in CT. As a result, it is important to keep the subcooling in the moderator. It is one of the major concerns in the CANDU safety analyses to estimate the local subcooling margin of the moderator inside the calanria tank. Previous experimental studies [1] showed that the film boiling would be unlikely to occur if the local moderator subcooling is sufficient. Therefore, an accurate prediction of the moderator temperature distribution in the calandria tank is needed to confirm the channel integrity [2].

There have been numerous computational efforts to estimate the thermal hydraulics in the calandria tank using CFD codes. Hadaller *et al.* [3] obtained a tube bank pressure drop model for tube bundle region of the calandria tank and implemented it into the MODTURC_CLAS code. Yoon *et al*. [4] used the CFX code to develop a CFD model with a porous media approach for the core region. However, it is known that porous media modeling provide only average values of flow velocities and temperatures and do not give any information about local flow variables near tube solid walls, which are necessary to implement accurate heat transfer calculations [5].

Recently, porous media modeling in the tube bank region of core using economic computing resources are replaced by the full geometric model of calandria tubes requiring high computing resources.

In this study OpenFOAM (Open Field Operation and Manipulation) [6], an open source CFD solver, is used to simulate the three-dimensional moderator flow in calandria tank of CANDU-6 reactor improving the computational efficiency by parallel computing which does not need any proprietary license.

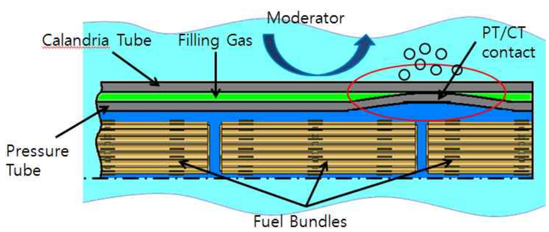


Fig. 1. PT/CT ballooning contact and moderator cooling.

2. Simulation Methods

2.1 OpenFOAM Setups

OpenFOAM (Open Field Operation and Manipulation) has been developed by Henry Weller and Hrvoje Jasak in Imperial College. The source code has been opened to the public since 2004. This code is operated on the Linux based O/S such as Ubuntu, so the copyright is absolutely free for every CFD program developer. This code is originated from the OOP (object oriented programming) concept based on C++ program language. Solvers and libraries are defined as C++ classes. With the post processor ParaView, the graphical visualization becomes possible with a command paraFoam [6].

In this study OpenFOAM vesersion 2.3.0 is used. The numerical calculations are conducted with two OpenFOAM standard solver, buoyantBoussinesq-SimpleFoam and buoyantBoussinesqPimpleFoam. The governing equations of the solvers are incompressible continuity equation, the Navier-Stokes equations and heat transfer equation. The buoyant force was calculated by Boussinesq approximation. For the turbulent flow in the moderator, k-ε turbulence model is also applied. buoyantBoussinesqSimpleFoam is for steady flow the velocity and pressure are coupled with SIMPLE algorithm and buoyantBoussinesqPimpleFoam is for unsteady flow the velocity and the pressure are coupled with PIMPLE algorithm.

2.2 Governing Equations and Discretization

The hydraulic governing equations based on the single-phase incompressible flow are written in the vector form:

$$\nabla \cdot \mathbf{V} = 0 \tag{1}$$

$$\rho\left\{\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V}\cdot\nabla)\mathbf{V}\right\} = -\nabla p + \rho\mathbf{g} + (\mu + \mu_t)\nabla^2\mathbf{V} + \mathbf{f}_V \tag{2}$$

where $\mathbf{V}$, ρ , p are velocity vector, density, and pressure while the constants μ and $\mathbf{f}_V$ are dynamic viscosity and body force per unit volume. Eq. (1) is the continuity equation for incompressible flow, and the Navier-Stokes momentum equation, Eq. (2) is decoupled from energy equation in the source term, or buoyancy force of Boussinesq approximation, $\mathbf{f}_V \approx -\rho\mathbf{g}\beta(T - T_0)$, where β is the thermal expansion in the unit of $1/K$, and $T - T_0$ is the difference of temperature from the reference condition.

A standard $k-\varepsilon$ model is used for the simulation of turbulent flow. This model includes two additional equations in a tensor form:

$$\rho\left\{\frac{\partial k}{\partial t} + (\mathbf{V}\cdot\nabla)k\right\} = \frac{\partial}{\partial x_j}\left\{\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right\} + P_k + P_b - \rho\varepsilon - Y_M + S_k \tag{3}$$

$$\rho\left\{\frac{\partial \varepsilon}{\partial t} + (\mathbf{V}\cdot\nabla)\varepsilon\right\} = \frac{\partial}{\partial x_j}\left\{\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right\} + C_{1\varepsilon}\frac{\varepsilon}{k}\{P_k + C_{3\varepsilon}\max(P_b, 0)\} - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} + S_\varepsilon \tag{4}$$

In Eqs. (3)~(4), the turbulent eddy viscosity is defined as:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{5}$$

where Eq. (5) is substitute to Eq. (2) for the consideration of turbulence.

Other coefficients in Eqs. (3)~(4) are listed as follows:

$$C_{1\varepsilon} = 1.44,\ C_{2\varepsilon} = 1.92,\ C_\mu = 0.09, \quad \sigma_k = 1.0,\ \sigma_\varepsilon = 1.3 \tag{6}$$

The energy equation to get the temperature field for the computation of $\mathbf{f}_V$ in Eq. (2) is

$$\rho C_p\left\{\frac{\partial T}{\partial t} + (\mathbf{V}\cdot\nabla)T\right\} = \left(\lambda + \frac{\mu_t}{\mathrm{Pr}_t}C_p\right)\nabla^2 T + Q_s \tag{7}$$

where T is temperature; C_p is heat capacity; λ is thermal conductivity; Pr_t is turbulent Prandtl number, set to simply 0.9 for most of fluids, and Q_s is volumetric heat source.

The convection terms of the governing equations are discretized with 2nd order upwind scheme and diffusion terms are calculated with 2nd order centered difference scheme. Turbulence equations and heat transfer equation were discretized with first order upwind scheme.

In the computation using OpenFOAM, SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm, a kind of FVM is applied for the iteration until the steady state for Eqs. (1) and (2). In this method, the pressure gradient term in Eq. (2) is isolated, and sub-iterations should be performed between predictor and corrector [7]. The PISO (Pressure Implicit with Splitting of Operator) SIMPLE or PIMPLE method is used for unsteady time marching, which is specified as no under-relaxation and multiple corrector steps in the calculation of momentum. PIMPLE is far accurate in time, and applied to the unsteady computation instead of SIMPLE.

2.3 Boundary and Initial Conditions

The essential boundary conditions in this problem are listed as follows:

- Velocities: no-slip conditions at walls, and the mass flow rate is specified on the inlet, fixed to 127.4 kg/s per each inlet nozzle, or 1019 kg/s in total for the present problem;
- Pressure: zero pressure gradient conditions at walls and inlet, which should be valid under the assumption that the thickness of boundary layer is very thin. The outlet pressure is fixed by the moderator system.
- Temperature: the inlet temperature is fixed to $47.3\,^oC$.

Total thermal power exerted to the whole system is 100 MW, which should be processed as the source term, Q_s in Eq. (7) where the factor 1.088742 should be multiplied, due to the volume occupied by the bundle of tubes. The equivalent temperature, or the energy dived by density and heat capacity, should be considered in the energy equation of OpenFOAM where the temperature should be specified instead of power. The power distribution is defined as $Q_s(r,t) = Q_s f_1(r) f_2(z)$, and the shape functions are, in the dimensionless form,

$$\begin{aligned} f_r(r) &= 0.94588 - 0.01989r + 0.0995r^2 \\ &\quad - 0.03888r^3 - 0.00256r^4 \ (0.0 \le r \le 3.38\ m) \\ f_z(z) &= 1.0 - 0.1111z^2 \ (-3.0 \le z \le -3.0\ m) \end{aligned} \tag{8}$$

The initial temperature of the whole computational domain is 47.3 ^oC , and the flow is stationary in the beginning of computation.

The properties of the fluid (D_2O) for the simulation are summarized in the Table I.

Table I: Material Properties of the Heavy Water

Definition (Symbol)	Value/Unit
Density (ρ)	1085 kg/m^3
Thermal expansion (β)	5×10^{-4} K^{-1}
Dynamic viscosity (μ)	5.5×10^{-4} kg/(m-s)
Heat Capacity (C_p)	4207 J/(kg-K)
Thermal conductivity (λ)	0.659 W/(m-K)

2.4 Grid Generation

The prototype of CANDU-6 is such as Fig 2. The 380 circular rods called calandira tubes are allocated symmetry from the central line of tank; the inlet holes are four along each side part, i.e. eight in total; and there are two outlet exits at the bottom. This prototype has an asymmetric shape along the longitudinal direction.

Fig. 2 also shows the three-dimensional grids at the view of lateral and longitudinal direction. The circular parts of calandria tubes and tank wall are bounded with structural grids, and hexahedral unstructured grids are used in the interfaces. As the shape is complicated in the inlet and the outlet, those parts are composed of tetrahedral unstructured grids. Though the types of grids are different, pyramid shape grids shares the boundary nodes of dissimilar shapes to suppress numerical error often brought out in the process of interpolation. The total grids are 6,740,446 consisting of 5,112,270 for the hexahedral, 13,112 for pyramids, and 1,615,064 for the tetrahedral. They are concentrated at the wall boundary to increase the accuracy in turbulent boundary layers.

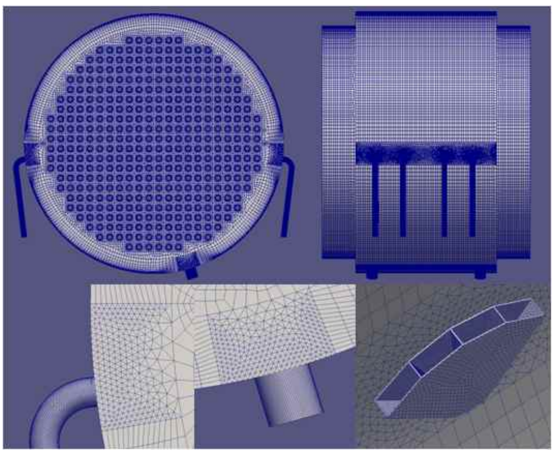


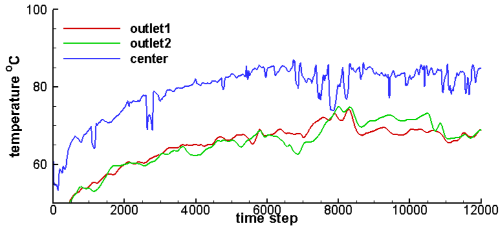
Fig. 2. Grids of the prototype: (from right upper, counterclockwise) side longitudinal, planform sectional, inlet plumbing, outlet exit, and feeding nozzle.

3. Result and discussions

3.1 Quasi-Steady State

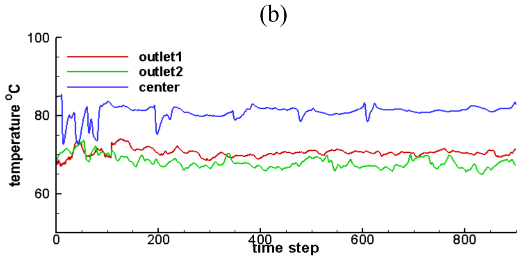
The solution is not converged to a steady state, but instead it fluctuates with oscillation. In the earlier stage, steady solution is obtained with SIMPLE algorithm. After the computation is stabilized, in the later stage, the solution is time marched to get the unsteady one. Fig. 3 is the temperature at two outlets and the origin of (a) quasi-steady before 12,000 time steps and (b) unsteady procedure.

The temperature of two outlets are slight different from each other because of the asymmetry from flow instability. At the center, the time-averaged temperature is 89 ^oC .



(a) Earlier stage, or steady solution

(b)



(b) Later stage, or unsteady solution

Fig. 3. Temperature at two outlets and center.

3.2 Turbulent Scale

To show how the grid system in Fig. 2 can capture turbulent physics in a proper scale, the normalized wall distance, y^+ is plotted in Fig. 4, which is ranged widely. However, with the use of the wall function, the value of $y^+ < 80$ should be enough in the most of computational domain of the present problem.

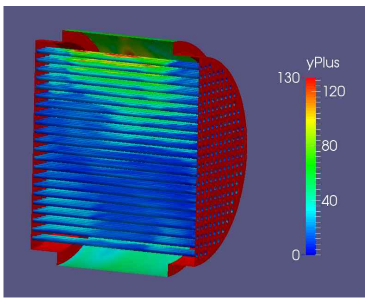


Fig. 4. Distribution of y^+ at 935 s.

3.3 Unsteady Solution

After the quasi-steady state, the time is started to counted, and the fields of velocity and temperature are visualized in Figs. 5~8 from 685 to 935 seconds.

Figures 5 and 6 are plotted at the sectional plane $z=0$, and the change of velocity and temperature are observed in the series of figures, respectively. In Fig. 5, the cooling water from nozzles in both sides meets at a stagnation point in the upper right-hand side. The flow field seems to be periodic for 250 seconds time difference. However, the temperature field in Fig. 6 presents no obvious regularity. The period is not distinguished in the figures, but they are repeated with time passing. The flow velocity is very slow less than 1 m/s in most of the domain, and no local region is found for the rapid increase of temperature.

Figures 7 and 8 are plotted at the sectional plane $x=0$, and the flow is not converged, too. In Fig. 7, the flow velocity is so slow, but the marks of calandria tubes are dimly visible as they decelerate the circulation flow. The maximum temperature stays about $89\,^{o}C$ in Fig.8, and also cannot be found the region of continual increase of temperature.

The velocity distribution in Figs. 5 and 7 shows obviously that the flow circulation penetrates the interval of circular rods decelerating the flow with a pressure drop. The diffused flow makes the temperature increase at the central region in Fig. 6 because flow resistance takes the worse cooling efficient. In the temperature field view of Fig. 8, the turbulent eddies can be discerned at the interface of different temperature at the upper half plane. They merge and separate continuously, developing a highly complex turbulent structure. The thermal boundary layer is usually thicker than a momentum boundary layer in $\mathrm{Pr}<1$ flows, so the high temperature difference of about $20\,^{o}C$ is dramatically visualized in both Figs. 6 and 8.

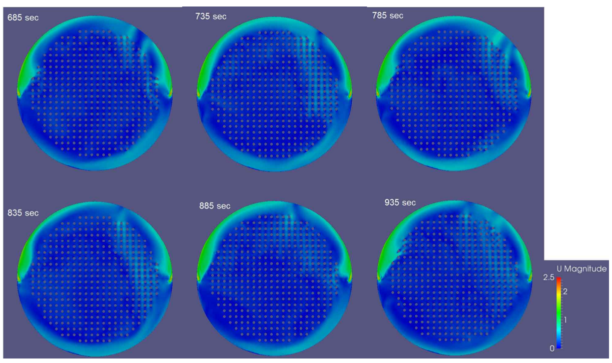


Fig. 5. Velocity distribution at z=0; 685~935 sec.

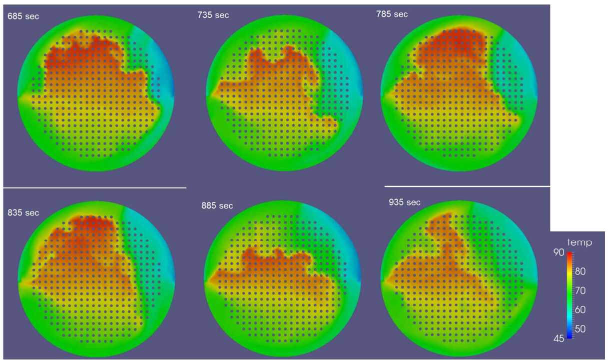


Fig. 6. Temperature distribution at z=0; 685~935 sec.

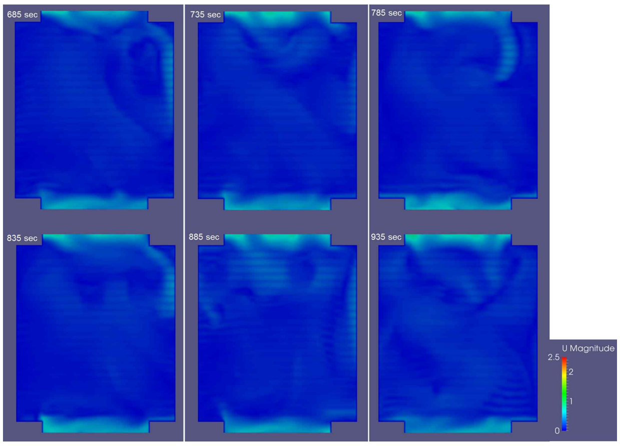


Fig. 7. Velocity distribution at x=0; 685~935 sec.

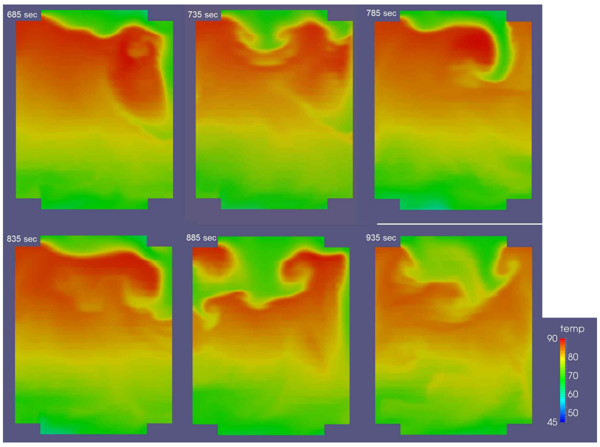


Fig. 8. Temperature distribution at x=0; 685~935 sec.

4. Conclusions

A prototype of CANDU-6 reactor is numerically analyzed about three-dimensional moderator flow in calandrian tank with OpenFOAM, an open source CFD code. The three-dimensional shape including 380 rods in the calandria tank is precisely modeled without porous approximation to avoid parasite errors. The buoyancy term in the incompressible Navier-Stokes equation is considered with Boussinesq approximation of the temperature variation. Turbulence effect is reflected to energy equation as well as momentum equation with $k-\varepsilon$ model.

The computational result shows that there should be no steady solution about the circulation flow, and therefore the unsteady simulation is achieved after getting a quasi-steady with oscillation of flow properties. Main findings on the present problem is listed as

(1) After 12,000 seconds from initial condition to the quasi-steady state, the unsteady simulation within 935 seconds shows no evidence of periodic oscillation for physical properties. The observation for 250 seconds presents a complex structure of turbulent mixing.
(2) There are not any regions where the temperature rises continuously due to very slow flow. Most of computational region marks the velocity less than 1 m/s. As the inlet nozzle flow going down from the stagnation point, it is highly diffused with the pressure drop due to the calandria tubes. Turbulent eddies were found in the temperature field, continuously developing to merge or separate at the interface of hot and cool fluid.
(3) For more precise analysis, the grid system have to be modified based on this calculation results and time-accurate unsteady flow analysis should be conducted. The dimensionless wall distance of the first grid from wall, y^+ was checked as less than 80 in the most of computational domain, but should be reduced with finer grids free of wall functions.

Overall, this research presents that the use of an open-source software is also very feasible for the application of analysis on the moderator system of PHWR such as CANDU-6. Compared with other commercial codes, the equivalent computation could be obtained from cheaper price and free copyright.

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