Validation of the MODTURC_CLAS Moderator Circulation Code for CANDU 9 Steady-State and Transient Conditions

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1. INTRODUCTION

Knowledge of the moderator flow and temperature distributions within the calandria vessel of a CANDU reactor is particularly important for the safety analysis of certain postulated accident scenarios where the moderator is required to provide a backup heat sink to the emergency core cooling system.

The CFD computer code, MODTURC_CLAS, is employed by the CANDU industry to predict moderator flow and temperature distributions in a range of CANDU moderator designs. It is based on the commercial general-purpose CFD code, TASCflow, developed by AEA Technology Engineering Software Ltd. (formerly Advanced Scientific Computing Ltd.) [1]. The code solves the coupled conservation equations of mass, momentum, thermal energy, turbulence kinetic energy and turbulence energy dissipation rate. Buoyancy effects are modelled using the Boussinesq approximation. The effect of the fuel channels is modelled by using a uniform isotropic porosity to account for the flow-volume reduction, and an empirically based friction-factor correlation to model the distributed hydraulic resistance to the mean flow.

In the recent CANDU 9 design (Figure 1), the moderator is introduced into the calandria vessel through a system of twelve downward-pointing nozzles located symmetrically on both sides of the calandria shell, at about the 10:45 o'clock position. Each nozzle is fitted with fan-shaped, multicompartment diffusers that emit flat, spreading jets of fluid in the reflector region, approximately parallel to the calandria wall. These jets meet at the bottom of the core at approximately the vessel's vertical plane of symmetry (the 6 o'clock position), and turn upward to flow through the core region to remove the heat generated by direct deposition of neutron and gamma energy to the moderator. The hot moderator fluid is removed via four outlet ports, symmetrically located on the vessel wall at approximately the 11:00 o'clock position, passed through external heat exchangers, and returned to the inlet nozzles.

This paper describes the validation of the MODTURC_CLAS code (version 2.2.1a) against data from the Moderator Test Facility (MTF), designed to simulate representative CANDU 9 steady-state and transient moderator flow conditions.

2. MTF SCALING CONSIDERATIONS

To validate the MODTURC_CLAS code, it is desirable to use data from experiments that relate, as far as possible, to the actual geometry and processes occurring within the moderator. The MTF was designed and built to conduct such experiments. It is an integral test facility, having all the key characteristics of a typical CANDU reactor calandria vessel, with all linear dimensions being ¼ of the corresponding physical values in the CANDU 9 reactor [2].

The scale was arrived at by balancing two competing requirements. It had to be large enough to ensure turbulence throughout the vessel, so that all the governing phenomena in the full-scale reactor calandria play essentially the same role in the reduced scale. At the same time, the size had to be economically viable in terms of capital and operating costs, particularly in aspects related to power and flow requirements, which can increase dramatically with increased scale.

Once the scale was chosen, dimensionless groups, derived by non-dimensionalizing the governing equations, were used to select the appropriate MTF operating conditions to simulate the corresponding full-scale reactor conditions.

The moderator flow and temperature distributions are governed by the following dimensionless groups:

dimensionless volumetric heat source,

$$\overset{*}{Q} = \frac{QD}{rC_p V \Delta T} \tag{1}$$

Archimedes number, which characterizes the ratio of buoyancy to inertia forces,

$$Ar = \frac{gb\Delta TD}{V^2} \tag{2}$$

Reynolds number,

$$\mathrm{Re} = \frac{rVD}{m} \tag{3}$$

and Prandtl number,

$$\mathrm{Pr} = \frac{C_p m}{l} \tag{4}$$

Q* and *Ar* were exactly matched for the MTF and the CANDU 9 calandria vessel, as they were identified to be the primary similarity parameters in the MTF scaling. The thermophysical properties of light water in the MTF and heavy water in the reactor calandria are similar enough to result in close Prandtl numbers similarity. Because of the ¼ length scale chosen for the MTF, it was not possible to achieve Reynolds number similarity. However, as mentioned, the scale was chosen large enough to obtain turbulent flow throughout the MTF vessel (as later confirmed from flow visualization and measurement of turbulence intensities). It can be shown that under such conditions, the relative levels of turbulent mixing in the MTF and reactor calandria, as characterized by the non-dimensional momentum and thermal diffusivities, are virtually independent of the Reynolds number.

To minimize electric power requirements for the calandria tube heaters used to simulate the volumetric neutron and gamma heating in the reactor, the outlet-to-inlet temperature difference *DT* for the MTF was chosen to be 1/3 the reactor value. This was judged to be large enough to allow for sufficiently accurate temperature measurements, taking into account known measurement instrument errors. With this choice of

DT, the above equations for *Ar* and *Q** were used to calculate the total power and inlet flow rate in the MTF.

3. MODTURC_CLAS MODEL

3.1 Phenomena - Modelling Aspects

As mentioned, MODTURC_CLAS solves the time-averaged conservation equations of mass, momentum and energy, coupled with the standard *k-e* model of turbulence. The following is a brief description of modelling aspects of the key phenomena governing moderator circulation.

3.1.1 Moderator Buoyancy

Moderator buoyancy, resulting from density variations, is accounted for via the gravitational force term in the momentum equation, which acts in the vertical *z* direction. By redefining the pressure in the momentum equation as the sum of the static pressure and a hydrostatic component based on a reference density:

$$p = p_s + r_r g_z z \tag{5}$$

the buoyancy force per unit volume can be expressed as:

$$S_{b,z} = g\left(r - r_r\right)g_z \tag{6}$$

The density difference in the above equation can be expressed in terms of the corresponding temperature difference by introducing the volumetric thermal expansion coefficient calculated from:

$$b = -\frac{1}{r_r}\left(\frac{\partial r}{\partial T}\right)_p \cong -\frac{1}{r_r}\left(\frac{r - r_r}{T - T_r}\right) \tag{7}$$

Using the above to substitute for the density difference in Equation (6), the buoyancy force per unit volume becomes:

$$S_{b,z} = -g\, b\, r_r \left(T - T_r\right) g_z \tag{8}$$

The above linearization of the buoyancy term, known as the Boussinesq approximation, is used in the MODTURC_CLAS code. MODTURC_CLAS can accommodate either a constant or temperature-dependent thermal expansion coefficient. For the validation work reported herein, a constant value was used.

3.1.2 Turbulence and Inlet Jet Development

To model turbulence effects on moderator inlet jet development as well as on the overall flow in the core and reflector regions, MODTURC_CLAS uses the two-equation *k-e* model for turbulence, together with wall functions to account for boundary-layer effects near the wall. Turbulent Reynolds stresses and turbulent heat fluxes are then estimated using effective viscosities and thermal conductivities, multiplied by mean velocity and temperature gradients, respectively.

The effective viscosity is defined by:

$$m_e = m + m_t \tag{9}$$

where the turbulent viscosity is calculated from the turbulent kinetic energy and the energy dissipation rate using the relation:

$$m_t = c_m r_r \frac{k^2}{e} \tag{10}$$

The effective thermal conductivity is in turn calculated as the sum of molecular and turbulent components from:

$$l_e = l + l_t = C_p \left(\frac{m}{\mathrm{Pr}} + \frac{m_t}{s_t} \right) \tag{11}$$

The *k-e* model works well in flows with one dominant mechanism for generating turbulence. However, it has been established that the model is often deficient in complex flows in which other aspects are introduced, e.g., streamwise curvature (such as the calandria vessel wall), pressure gradients and buoyancy forces. The deficiencies are largely attributed to the formulation's direct relationship between the Reynolds stresses and the mean velocity gradient [3]. As well, because a porous media approach is used to model the effects of the calandria tubes (see below), the *k-e* model, as implemented in MODTURC_CLAS, does not account for any additional turbulence generated by the interaction of the moderator flow with the calandria tubes.

There are a number of empirical constants used in the *k-e* model. The recommended values are listed in the table below [3].

c_μ	$c_{1\varepsilon}$	$c_{2\varepsilon}$
0.09	1.44	1.92

Sensitivity studies have shown that predictions can be quite sensitive to the values of $c_{1\varepsilon}$ and $c_{2\varepsilon}$. For example, a 5% change in either constant can result in a 20% change in the spreading rate of a jet [3]. All analyses reported herein, except some sensitivity cases (see Section 4), were done using these values as defaults.

3.1.3 Interaction with Calandria Tubes

Because of limits to current computing resources, state-of-the art calculations of flows in large tube banks do not involve detailed calculations around individual tubes. Rather, the approach used in MODTURC_CLAS and other codes that model similar problems is to solve the governing partial differential equations over the domain and treat the core region as a porous medium. The latter is characterized by an isotropic porosity, to reflect the average reduction in local fluid volume, and a distributed resistance, to reflect the hydraulic skin friction and drag characteristics of the calandria tube array.

The isotropic porosity in the core region is calculated from:

$$g = 1 - \frac{p}{4} \left(\frac{d}{p} \right)^2 \tag{12}$$

The momentum sink per unit volume, to account for pressure losses in the calandria tube bank, is calculated from:

$$S_V = -\frac{1}{2}\frac{f}{l_{row}} r_r g^3 \vec{V} V f(\Psi) \tag{13}$$

in the above, the distance between tube rows is calculated from:

$$l_{row} = p\cos(a) \tag{14}$$

where a is the angle between the flow direction and either the horizontal or vertical component of the flow, whichever is dominant. For in-line flow, a is equal to 0.

The function $f(Y)$ is introduced to account for the pressure loss due to flow along the tube axis (i.e., parallel flow), which is lower than in cross-flow.

The cross-flow friction factor for the relatively large pitch-to-diameter ratio typical of CANDU calandria tubes, has been determined from tests on tubes arranged in in-line and staggered arrangements in the Stern two-dimensional moderator test facility [4]. It is given by

$$f = 4.5626\,\mathrm{Re}_{fs}^{-0.1655} \tag{15}$$

where Re_{fs} is the Reynolds number based on the tube diameter and free-stream or approach velocity:

$$\mathrm{Re}_{fs} = \frac{r_r V_{fs} d}{m} = \frac{r_r g V d}{m} \tag{16}$$

3.1.4 Energy Deposition in the Moderator

During normal operation of the reactor, thermal energy is deposited directly into the moderator liquid as the result of the slowing down of neutrons from the fission process, as well as the absorption of gamma rays and beta particles from fission products and various sources. The neutron heating component dominates during normal reactor operation; therefore the local volumetric heat generation rate is approximately proportional to the local neutron flux and, hence, reactor power. During a transient, such as a large LOCA, the neutron component rapidly decreases as the reactor is tripped, and the principal source of heating is from gamma rays due to fission product decay, along with heat transferred from the fuel channels and other components. The heat transferred from the fuel channels may become significant if pressure tube ballooning occurs. The energy deposition from any of the above processes is determined from physics and fuel channel calculations and modelled in MODTURC_CLAS by the specification of a volumetric heat generation rate in the energy equation:

$$S_T = f(Q, x, y, z, t) \tag{17}$$

In the MTF, energy deposition to the moderator fluid is simulated by the direct electrical heating of the calandria tubes, with the heat transferred to the light-water coolant, representing the heavy-water moderator, by a combination of natural and forced convection. The details of the heat transfer process from the individual calandria tube surfaces to the coolant are not modelled; instead, the local deposition of thermal energy from the electric heating is included as a local volumetric heat source (i.e., Equation (17)), the same way as in an operating reactor.

3.2 Boundary Conditions

Boundary conditions are as follows: at the inlets, a uniform fluid velocity, temperature, k and e are specified; at the outlets, the pressure is given; and at the vessel walls, the no-slip adiabatic conditions are used. The values of k and e at the inlets are expressed in terms of the inlet turbulence intensity and the eddy length scale, taken as being 0.05 and 0.005 m, respectively.

3.3 Computational Grid and Solution

The computational grid used is the butterfly design grid (see Figure 2). The base grid applied in most simulations comprises 69x82x24 = 135 792 nodes, with 69 being the number of cross-sectional planes in the axial direction, and 82x24 = 1968 being the number of nodes in each cross-sectional plane. The base grid size was chosen based on the results of grid independence tests involving three other nodalizations, two finer than the base grid, and one coarser.

The MODTURC_CLAS equations are solved by iterations until user-specified convergence criteria are satisfied.

4. Results and Discussion

In all, the MTF was used to carry out five steady-state and two transient integral tests. The steady-state tests covered a range of possible steady-state operating conditions, including isothermal, nominal flow and power for two outlet-to-inlet temperature differences, nominal flow and power with inlet flow asymmetry, and reduced flow and power with inlet flow asymmetry to simulate one-pump operation. The transient tests were designed to simulate, in a stylized way, the main features of two postulated accident scenarios: a large LOCA with LOECC (Loss Of Emergency Core Cooling), and a large LOCA with loss of Class IV power. Measurements during the steady-state tests included local velocities (magnitudes and turbulence intensities) and temperatures throughout the vessel using moveable probes, whereas measurements during the transients were limited to coolant temperatures throughout the vessel using fixed probes.

All of the above tests were simulated and assessed with MODTURC_CLAS. In addition a number of additional simulations of the nominal steady state flow and power test were carried out to investigate sensitivity of flow and temperature predictions to grid spacing; reduction of nozzles flow areas; and changes to the turbulence model constants, hydraulic resistance of the calandria tube bank, and axial variation of the volumetric heating rates.

Figures 3 and 4 compare predicted and measured temperature distributions and velocity vectors in the middle cross-section of the MTF vessel for the steady-state test with nominal flow and power conditions. The figures illustrate the typical patterns of flow and temperature distributions in the MTF core: the fluid flow is predominantly vertical and the temperature distribution is stratified, i.e., the fluid temperature increases with elevation. The asymmetry in the velocity measurements at the vessel bottom is attributed to a combination of the highly unsteady nature of the turbulent jets and possible geometric misalignments of the inlet nozzles due to manufacturing tolerances. Code predictions do not show this asymmetry because the k-e model accounts for only the mean behaviour of the turbulent flow and not its unsteady nature, and the nozzle geometries on each side of the vessel were assumed symmetric.

Figure 5 shows good agreement between the predicted and measured time-variation of the liquid temperature in the upper part of the core during the stylized large LOCA+LOECC experiment.

In general, the code predictions, particularly the location and magnitude of the maximum temperature, were found to be relatively insensitive to the changes in the parameters investigated, with one exception. Figure 6 shows that better agreement between measured and predicted temperatures in the lower part of the core is obtained when the turbulence model parameter c_{1e} is decreased by 10% and c_{2e} is increased by 10%. These results suggest that the use of the default parameters in the k-e model leads to calculated jet entrainments that are too low, and, hence, result in the consistent underprediction of temperatures in the lower part of the vessel. A possible reason is that the interaction of the jets with the calandria tubes, which is not accounted for in the k-e model, could lead to more entrainment of core fluid by the jets.

Overall, results from the validation of MODTURC_CLAS against the MTF data for representative CANDU 9 steady-state and transient conditions indicate good agreement between the code predictions and measurements, specifically:

- The measurements and code predictions of velocity and temperature fields confirm the stability of the CANDU 9 moderator system over a wide range of conditions, including significant flow asymmetry resulting from one-pump operation.

- The measurements and code predictions show the temperature to be monotonically increasing from the bottom to the top of the core (Figure 3). In general, there is good agreement between the measured and predicted temperatures. There is a slight tendency to underpredict temperatures at the bottom of the vessel, possibly due to insufficient jet entrainment, as modelled by the code. However, agreement improves near the top, where the maximum temperature is reached. The difference between the predicted and measured maximum temperatures is less than 1°C.

- The measurements and code predictions indicate that the overall flow and temperature patterns are determined primarily by the forced flow induced by the inlet jets, as they flow and entrain core liquid toward the bottom of the vessel, collide, and induce a stable upward flow through the core, assisted by buoyancy forces (Figure 4).

- The measurements and code predictions indicate that the temperature field and, to a lesser extent, the velocity field are largely two-dimensional in the core cross-section, with decreasing axial variation as the top of the core is reached.

5. CONCLUSIONS

- The CFD code, MODTURC_CLAS, has been validated against MTF data representing a range of CANDU 9 nuclear reactor conditions.

- Good quantitative agreement between the code predictions of three-dimensional water temperature distribution in the MTF vessel and the temperature measurements has been obtained for both steady-state and transient simulations.

- The predicted and measured flow and temperature distribution patterns in the MTF vessel have confirmed the stability of the CANDU 9 moderator system.

6. ACKNOWLEDGEMENTS

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7. NOMENCLATURE

Ar	=	Archimedes Number
C	=	specific heat at constant pressure
d	=	calandria tube diameter
D	=	calandria vessel diameter
f	=	tube bank friction factor
g	=	gravitational constant
l	=	distance between tube rows
k	=	turbulent kinetic energy
p	=	pressure; pitch
Q	=	volumetric heat sources
Pr	=	Prandtl number
Re	=	Reynolds number
S	=	volumetric source term
t	=	time
$\vec{V}$, V	=	velocity vector and magnitude
z	=	co-ordinate along the vertical direction
a	=	angle
b	=	coefficient of volume expansion
e	=	energy dissipation rate
g	=	isotropic porosity
l	=	liquid thermal conductivity
m	=	liquid dynamic viscosity
s	=	turbulent Prandtl number
ρ	=	liquid density

Subscripts

b	=	buoyancy
e	=	effective
fs	=	free stream
r	=	reference
s	=	static
t	=	turbulent
V	=	velocity

z	=	vertical z direction
T	=	temperature

8. REFERENCES

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3. W. Rodi, *"Turbulence Models and Their Application in Hydraulics – A State of the Art Review,"* University of Karlsruhe Report SFB 80/T/127, 1978 May.

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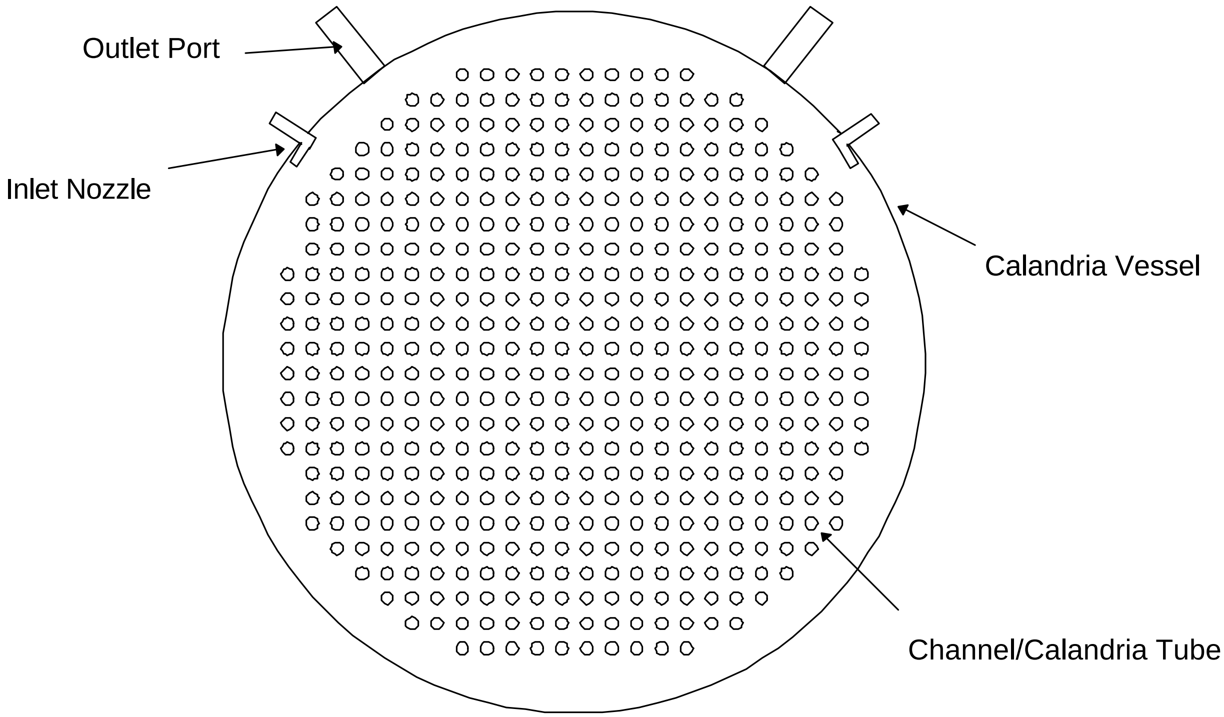

Figure 1: Simplified cross-sectional view of a CANDU 9 calandria vessel

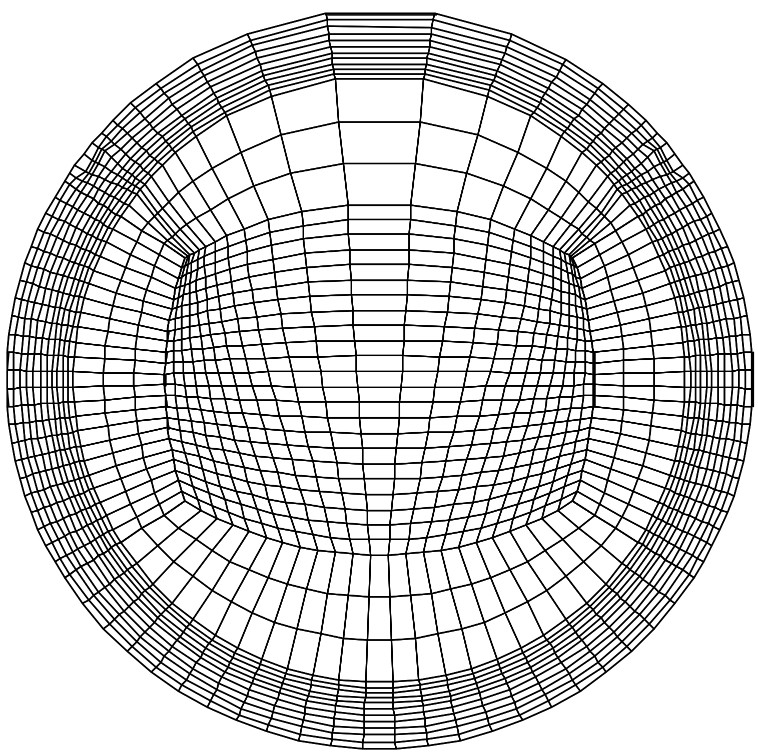

Figure 2: Cross-section of base grid at inlet nozzle plane

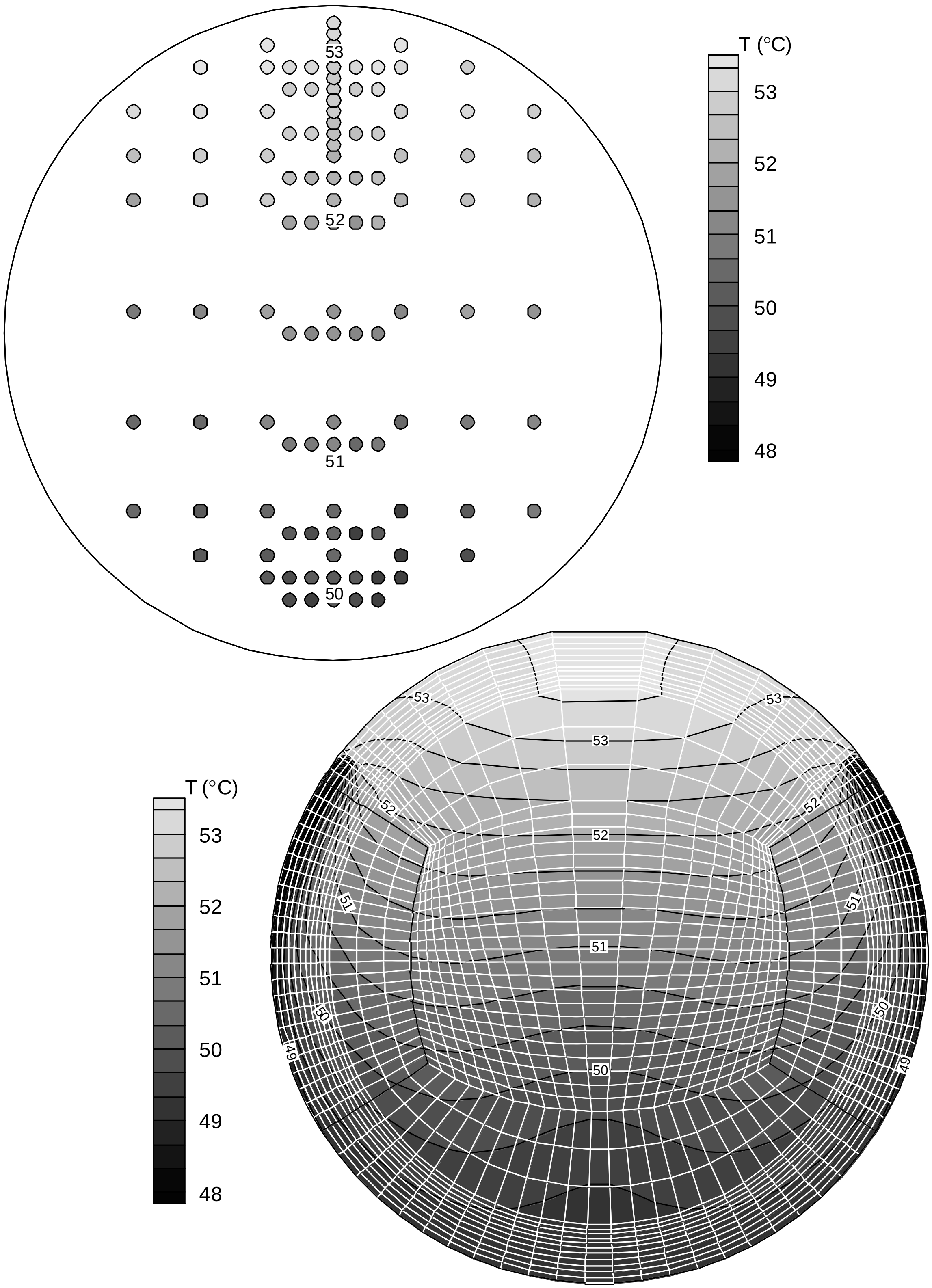

Figure 3: Comparison of predicted (lower) and measured (upper) temperature distributions in middle cross- section for nominal flow and power conditions

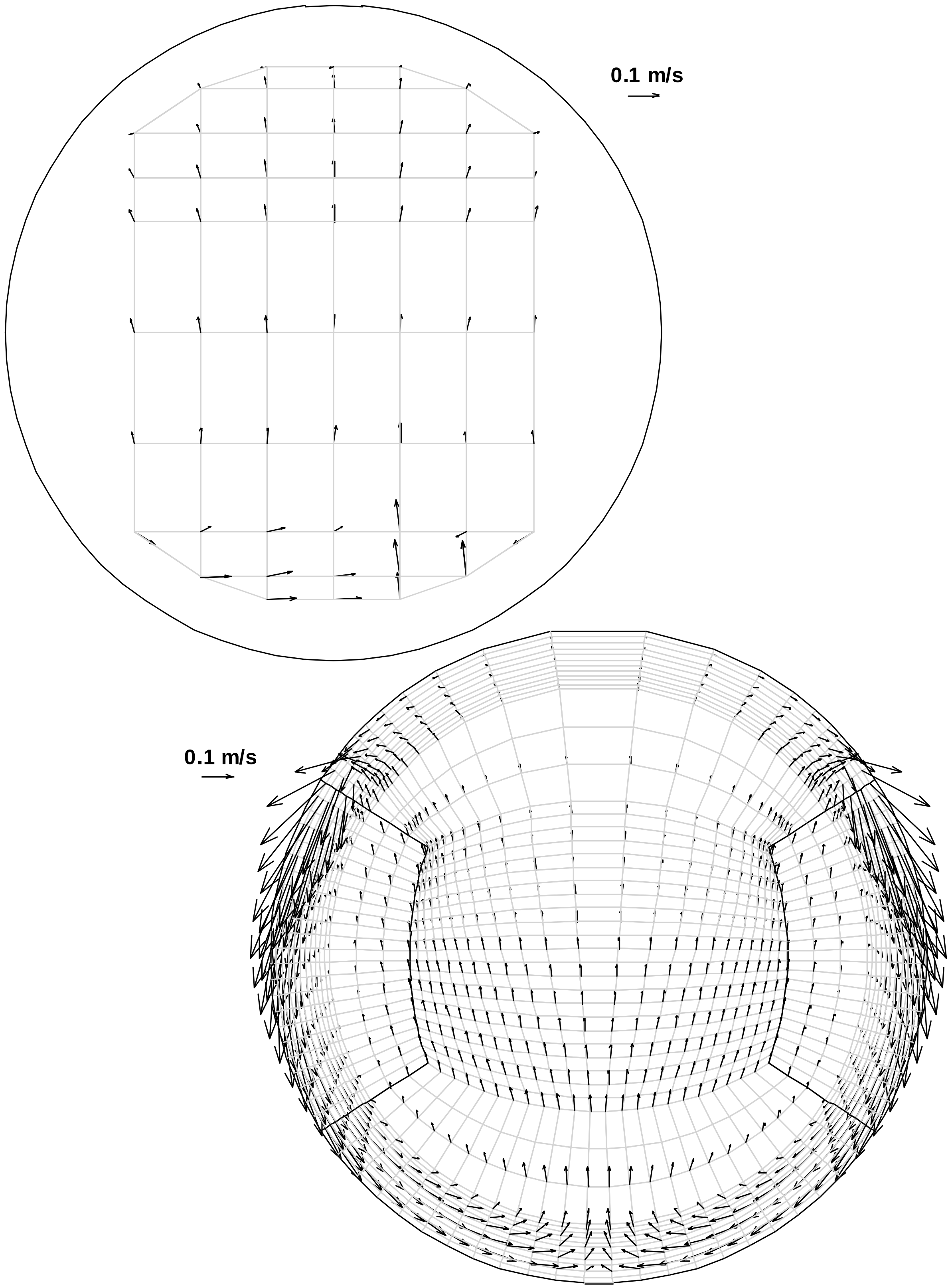

Figure 4: Comparison of predicted (lower) and measured (upper) velocity vectors in middle cross-section for nominal flow and power conditions

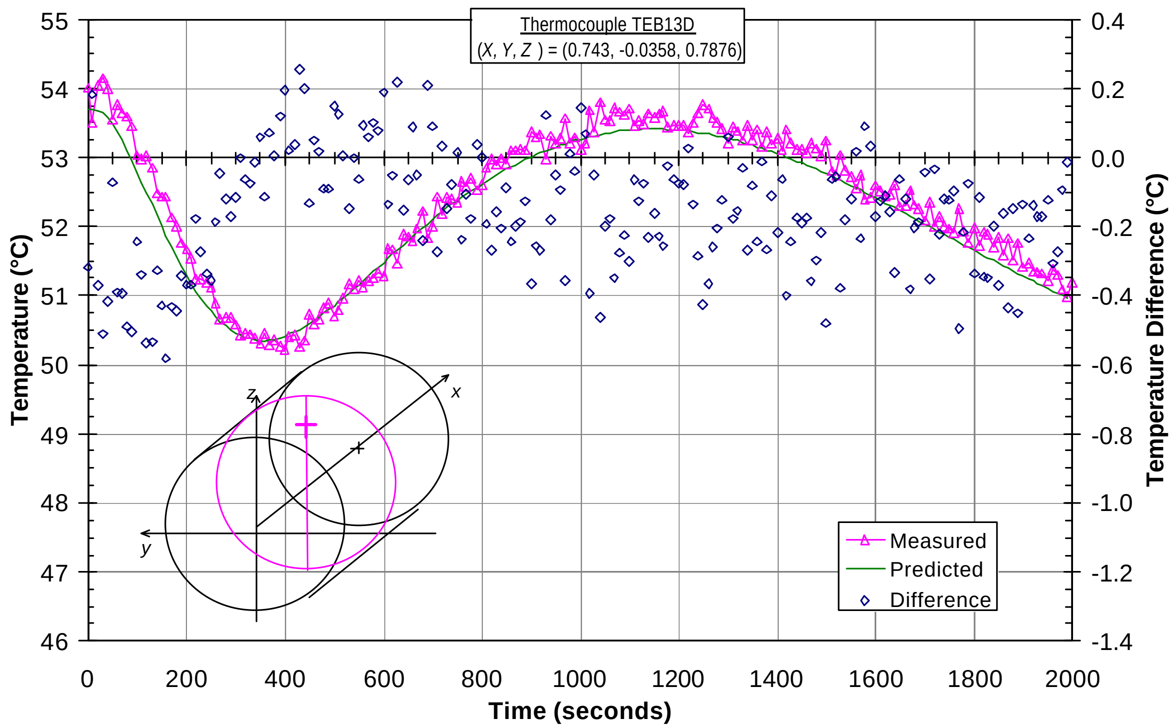

Figure 5: Predicted and Measured (gap thermocouple)Temperatures Near Top of Core for the Stylized Large LOCA+LOECC Transient.

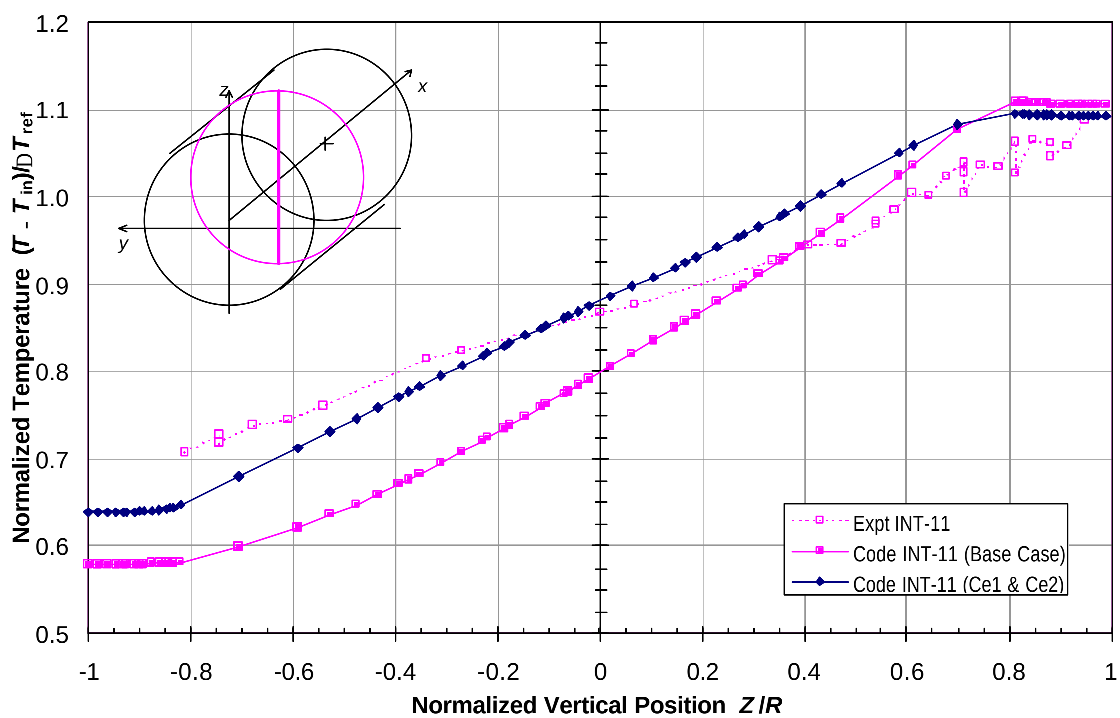

Figure 6: Predicted (Base Case and 0.9$c_{1\varepsilon}$, 1.1$c_{2\varepsilon}$) and Measured Temperatures Along Vertical Centerline for Nominal Flow and Power Test.