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Numerical models to predict steady and unsteady thermal-hydraulic behaviour of supercritical water flow in circular tubes

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HIGHLIGHTS

- A CFD model and 1-D code THRUST are developed to simulate the supercritical water flows.
- The supercritical flows with the normal heat transfer and deteriorated heat transfer are simulated.
- The numerical results are compared with the experimental data and the errors are reported.
- The transient simulations are also carried out using the CFD and THRUST.
- The transient results obtained using the CFD and THRUST are compared under different conditions.

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ABSTRACT

The present paper is aimed at the development of numerical models to predict steady and unsteady thermal-hydraulic behaviour of supercritical water flow at various operating conditions. A simple one-dimensional numerical thermal-hydraulic model based on a finite-difference scheme has been developed. A detailed CFD analysis based on two turbulence models, Reynolds Stress Model and $k-\omega$ SST model, has also been presented in this paper. Seven experimental cases of steady state and vertically up flowing supercritical water in circular tubes operated at various working regimes, such as normal and deteriorated heat transfer regions, are used to validate the numerical models. Comparisons for steady state flow show good agreement between the numerical and experimental results for all normal heat transfer cases and most of the deteriorated heat transfer cases. Next, the numerical models are used for transient simulations. Three case studies are undertaken with a purpose to quantify the time dependent responses from both the 1-D model and CFD model. The comparisons carried out for both the normal and deteriorated heat transfer conditions show a good agreement between the two numerical models.

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1. Introduction

The supercritical water cooled reactor (SCWR) has been identified as one of the six proposed technologies for the generation IV nuclear reactors (U.S. DOE NERAC and GIF, 2002) because of its advantage of high thermal efficiency, compact plant system, avoidance from boiling crisis and close proximity to the proven technology of supercritical fossil power plants. Therefore, the SCWR has received attention among the researchers of various disciplines at present. The fluid flow and heat transfer characteristics and the

thermo-physical properties of various substances, such as water and CO₂, at supercritical conditions have been studied extensively since 1950s, such as the experimental research works carried out by Yamagata et al. (1972), Swenson et al. (1965), Jackson (2002) and many more as mentioned in the review papers by Duffey and Pioro (2005), Pioro et al. (2004) and Jäger et al. (2011). However, there are still issues need to be addressed in order to meet the present demand of making the SCWR technologically viable and economically feasible with adequate safety margin and to predict its behaviour accurately at normal and anticipated accidental operating situations.

In addition to the numerous experimental studies, economically attractive alternatives, the numerical approaches have been used extensively in recent years to get detailed insight into the heat transfer mechanism in supercritical fluids. In numerical studies, two approaches can be used – (i) CFD models and

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Nomenclature

a	acoustic speed, m/s
A	area, m ²
c_p	specific heat capacity at constant pressure, J/kg K
$\bar{c}_p$	$(h_w - h_b)/(T_w - T_b)$, J/kg K
D	diameter of a tube, m
e	specific internal energy, J/kg
g	gravitational acceleration, m/s ²
G	mass flux, kg/m ² s
h	specific enthalpy, J/kg
h_b	heat transfer coefficient, W/m ² °C
k	turbulence kinetic energy, m ² /s ²
L	length, m
L_h	heated length, m
p	pressure, Pa
P_H	heated perimeter, m
P_w	wetted perimeter, m
q_w	wall heat flux, W/m ²
r	distance from the centre of the tube, m
r^*	non-dimensional radial location
t	time, s
T	temperature, °C
u	velocity, m/s
W	mass flow rate, kg/s
y	distance from the wall, m
y^+	non-dimensional distance from the wall, $u_\tau y/\nu$, m
z	axial location, m
z^*	non-dimensional axial location

Greek letters

α	thermal expansion coefficient, 1/K
ϵ	energy dissipation per unit mass, m ² /s ³
λ	thermal conductivity, W/mK
μ	dynamic viscosity, Pa s
ν	kinematic viscosity, m ² /s
ρ	density of a fluid, kg/m ³
τ	shear stress; τ_w , wall shear stress, N/m ²
ω	specific dissipation rate, 1/s

Subscripts

b	bulk
cr	value at critical point
dht	deteriorated heat transfer
ex	exit
exp	experimental data
f	values at film, reference values between $y=0$ and $y=y$
in	inlet
m	mean
num	numerical
pc	pseudo-critical
q	based on local heat flux value
t	turbulent
w	wall

Dimensionless numbers

Bu^*	Buoyancy parameter, $\bar{Gr}_b/Re_b^{2.7} \bar{Pr}_b^{0.50}$
$\bar{Gr}_b$	$g(1 - \rho_w/\rho_b)D^3/\nu_b^2$
Nu	Nusselt number
Pr	Prandtl number, $\mu c_p/k$
$\bar{Pr}$	$\mu \bar{c}_p/k$
Re	Reynolds number, $\rho u D/\mu$

Acronyms

AECL	Atomic Energy of Canada Limited
BC	boundary condition
BWR	Boiling water reactor
CFD	computational fluid dynamics
DHT	deteriorated heat transfer
HTC	heat transfer coefficient
HTCD	heat transfer coefficient by Dittus–Boelter
HTCJ	heat transfer coefficient by Jackson et al.
HTCM	heat transfer coefficient by Mokry et al.
HTCS	heat transfer coefficient by Swenson et al.
HTCW	heat transfer coefficient by Watts et al.
MAE	mean absolute error
NHT	normal heat transfer
PCR	pseudo critical region
RSM	Reynolds Stress Model
SCR	supercritical reactor
SCW	supercritical water
SCWR	supercritical water cooled reactor
SD	standard deviation
SST	shear stress transport
TH	thermal-hydraulic
THRUST	Thermal-Hydraulic solveR Undertaking Supercritical waTer
TKE	turbulence kinetic energy

(ii) one-dimensional thermal-hydraulic (TH) models. The former approach is computationally expensive and its main challenge is to implement the accurate turbulence models for supercritical fluids. However, it can provide detailed information on the flow and heat transfer in all the directions. While the latter approach, which takes into account the axial variation of flow and thermodynamic properties, and averages the quantities along radial and azimuthal directions, is computationally efficient, flexible and may have the required accuracy if the empirical heat transfer correlation (HTC) are implemented properly.

Earlier numerical studies for supercritical flows using CFD models were done by [Desissler \(1954\)](#) and [Shiralkar and Griffith \(1969\)](#) using the turbulence models based on eddy diffusivity assumption. With the development of two equation turbulence models, $k-\epsilon$ and $k-\omega$ type turbulence models have been validated for the fluid flow and heat transfer investigation for supercritical fluids. Later, the $k-\omega$ SST model developed by [Menter \(1993\)](#) which combines the strength of $k-\epsilon$ model in free stream region and strength of $k-\omega$ in recirculating regions is used by various researchers, such as [Cheng et al. \(2007\)](#) and [Palko and Anglart \(2007, 2008\)](#). However, there is no common consensus among researchers regarding the capability of $k-\omega$ SST model for studying the heat transfer phenomenon in supercritical fluid flows. Therefore, in the current study, $k-\omega$ SST model will be used to assess its capability in predicting supercritical fluid flows under various operating conditions. It is important to note that the two-equation turbulence models are developed with the isotropic assumption. The researchers have also used anisotropic turbulence models such as the Reynolds Stress Model (RSM) for supercritical water flows in various geometries ([Zhang et al., 2011](#); [Cheng et al., 2007](#)). It was concluded from these studies that anisotropic turbulence models give better agreement with experimental results than other two-equation models with an isotropic assumption for the chosen experimental conditions. As turbulence models are sensitive to operating conditions, in the current study, the turbulence model RSM is also evaluated against experimental data to assess its capability under different

operating conditions. The CFD simulations are carried out using the commercial software Ansys FLUENT 14.5.

There are several 1-D TH models, such as those developed by Chatoorgoon (2001), Chatoorgoon et al. (2005a,b), Ambrosini and Sharabi (2008), Gómez et al. (2008) and Jain and Sharabi (2008). But those models were mainly used to predict the static and dynamic instabilities of supercritical reactors (SCRs) without giving much attention to evaluate their capability in predicting the wall temperature. The predicted wall temperature using the 1-D model depends on the empirical HTCs used in the model. Moreover, there are umpteen number of HTCs available in the literature which are experiment specific and thus, need validation before using them with TH model.

The reviews conducted by several authors (Pioro et al., 2004; Cheng and Schulenberg, 2003; Yoo, 2013) showed that the numerically predicted wall temperature is in good agreement with the experimental data mainly for the normal heat transfer (NHT) cases. However, for the deteriorated heat transfer (DHT) cases which are characterized by a sharp increase in the wall temperature, the numerical predictions are found to be challenging. Therefore, the numerical models presented in this study will be validated for both NHT and DHT cases.

The in-house 1-D Thermal-Hydraulic solver Undertaking Supercritical waTer (THRUST), which is an extension of an earlier version used for simulating boiling water reactor (BWR) (Dutta and Doshi, 2009), is used for the simulation of the SCWR in the present work. It is based on mass, momentum and energy conservation equations and includes the thermodynamic equation of state to take care of the property changes due to the pressure and temperature.

In this study, the THRUST and CFD models are evaluated by comparing the simulation results with the experimental data under various operating conditions. Further, both the numerical models are then used to simulate the transient response of the SCWR. Subsequently, the step change and periodic variation of various physical variables are introduced with a purpose to assess the capability of the numerical models to predict the heat transfer phenomenon during a transient process.

2. Mathematical details of the numerical models

The mathematical details of the THRUST and CFD models are presented in this section. The present analysis is carried out under both steady state and transient conditions.

2.1. Mathematical formulations of the 1-D TH model

In the 1-D THRUST, it is assumed that the thermo-physical flow properties vary along the axial direction only and the heat flux at the periphery of the circular tube is constant. The general fundamental one-dimensional governing equations for fluid flow and heat transfer are as follows:

Mass conservation equation:

$$\frac{\partial}{\partial t}(\rho A) + \frac{\partial}{\partial z}(\rho Au) = 0 \quad (1)$$

Momentum conservation equation in the axial direction:

$$\frac{\partial}{\partial t}(\rho Au) + \frac{\partial}{\partial z}(\rho Au^2) = -A \frac{\partial p}{\partial z} - \tau_w P_w - \rho Ag \quad (2)$$

Energy conservation equation:

$$\frac{\partial}{\partial t}(\rho Ae) + \frac{\partial}{\partial z}(\rho Aue_f) = q_w P_H \quad (3)$$

where $e = e_f - (p/\rho)$ and $e_f = h + (u^2/2) + gz$.

These equations can be written in a compact form as follows:

$$\frac{\partial}{\partial t}[\mathbf{R}] + \frac{\partial}{\partial z}[\mathbf{S}] = [\mathbf{T}] \quad (4)$$

where

$$\mathbf{R} = \begin{bmatrix} \rho A \\ \rho Au \\ \rho Ae \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} \rho Au \\ A(\rho u^2 + p) \\ \rho Aue_f \end{bmatrix}, \quad \mathbf{T} = \begin{bmatrix} 0 \\ p \frac{dA}{dz} - \tau_w P_w - \rho Ag \\ q_w P_H \end{bmatrix}$$

These governing equations in a conservative form are first converted into the following primitive form:

$$\frac{\partial}{\partial t}[\mathbf{U}] + \mathbf{A}(\mathbf{U}) \frac{\partial}{\partial z}[\mathbf{U}] = [\mathbf{D}(\mathbf{U})] \quad (5)$$

where $\mathbf{U}$ is a vector of unknown dependent variables $[W, h, p]^T$, $\mathbf{A}$ is a square matrix of coefficients which are functions of $\mathbf{U}$, and $\mathbf{D}$ is a vector containing allowances for mass, momentum, and energy to transfer across the system boundaries.

The equation of state, $\rho = \rho(p, h)$, is used and it is noted that all the thermodynamic properties in the present model are subjected to change depending on the pressure and enthalpy along the axial direction of the channel.

The eigenvalues of matrix $\mathbf{A}$ determine the mathematical class of Eq. (5) and it is found that all eigenvalues of $\mathbf{A}$ are real ($u, u+a, u-a$); and hence the governing equations are hyperbolic ones. Next, the set of Eq. (5) are transformed into a characteristic form and it can be written as the following:

$$\mathbf{B} \frac{\partial}{\partial t}[\mathbf{U}] + \mathbf{A} \frac{\partial}{\partial z}[\mathbf{U}] = [\mathbf{C}] \quad (6)$$

where $\mathbf{A}$ is a diagonal matrix of eigenvalues of $\mathbf{A}$.

After the coefficient and source term are linearized, Eq. (6) is discretized with a characteristics-dependent implicit finite-difference scheme where the spatial derivative terms are approximated by a backward or forward difference depending on the sign of the characteristics. For the present case of subsonic flows ($u < a$), the spatial derivatives for the first two governing equations, which are characterized by $\Lambda_{11} = u + a > 0$ and $\Lambda_{22} = u > 0$, respectively, are approximated by a backward difference equations and the third governing equation, which is characterized by $\Lambda_{33} = u - a < 0$, is approximated by forward difference equation. The resultant discretized equations are then combined together and used for a numerical solution depending on the boundary conditions for the particular problem.

2.1.1. Steady state solution methodology

The resultant discretized equations for Eqs. (1)–(3) for steady state flows are as follows:

$$\rho_{i+1} A_{i+1} u_{i+1} = \rho_i A_i u_i \quad (7a)$$

$$p_i - p_{i+1} = \frac{1}{2} \left(\frac{1}{A_i} + \frac{1}{A_{i+1}} \right) [(\rho Au^2)_{i+1} - (\rho Au^2)_i] + \frac{1}{2} [\{\rho(F+g)\}_i + \{\rho(F+g)\}_{i+1}] (z_{i+1} - z_i) \quad (7b)$$

$$(e_f)_{i+1} - (e_f)_i = \frac{1}{2} \left[\left(\frac{q_w P_H}{\rho Au} \right)_i + \left(\frac{q_w P_H}{\rho Au} \right)_{i+1} \right] (z_{i+1} - z_i) \quad (7c)$$

where $F = \tau_w P_w / \rho A$.

The above set of equations, in addition to the thermodynamic equation of state, are solved numerically by using a forward marching scheme when all the inlet primary variables, i.e., inlet velocity, enthalpy and pressure are specified, otherwise a shooting method

along with the forward marching scheme is employed to treat different set of specified boundary conditions.

2.1.2. Heat transfer coefficient and friction factor

The accuracy of such a 1-D TH model largely depends on appropriate selection of friction factor and HTC. In spite of extensive experimental investigations for last several decades, a common consensus in standardizing the use of general purpose HTC for various geometry and operating conditions at supercritical region is still not available. The commonly used HTCs by Dittus–Boelter (Incropera, 2011) (HTCD), Swenson et al. (1965) (HTCS), Watts and Chou (1982) (HTCW), Jackson (2002) (HTCJ) and Mokry et al. (2011) (HTCM) based on experimental data may be limited to specific conditions.

The simulations in this study are carried out by using Filonenko correlation (Kedzierski and Kim, 1994) for the friction factor and 5 different HTCs mentioned above. The numerical results using different HTCs will be compared with the available experimental data to verify their suitability and limitations. The study on the effect of the friction factor is not done in the present study because of lack of availability of relevant experimental results on pressure drop and its spatial distribution along the channel.

The 5 HTCs used in this study have the following form:

$$Nu_{\theta} = C \times Re_{\theta}^{n_1} Pr_{\theta}^{n_2} \bar{Pr}_b^{n_3} \left(\frac{\rho_w}{\rho_b}\right)^{n_4} \left(\frac{\mu_w}{\mu_b}\right)^{n_5} \left(\frac{\lambda_w}{\lambda_b}\right)^{n_6} \times \left(\frac{\bar{c}_p}{c_{pb}}\right)^{n_7} \phi \quad (8)$$

where $\phi = \phi(z, T_b, T_w, \dots)$ and the subscript θ represents b, w or f depending on whether the bulk temperature, T_b , wall temperature, T_w or mean film temperature, $T_f = 1/2(T_b + T_w)$, is used to determine the thermodynamic properties in the corresponding correlation. The parametric details of the 5 HTCs used in the 1-D model are listed in Table 1.

2.1.3. Methodology to determine the local wall temperature

The present study deals with the predefined heat flux at the circumference of the circular tubes. Therefore, all the thermodynamic variables representing the bulk properties of the SCW are obtained first by simultaneously solving the nonlinearly coupled steady state governing equations, i.e., Eqs. (7a)–(7c) and the thermodynamic equation of state. The calculation of Nu_{θ} using Eq. (8) depends on the wall temperature which is assumed first to start the calculation. Next, the heat transfer coefficient, h_b , and wall temperature, T_w , are determined by the following equations sequentially:

$$h_b = \frac{Nu_{\theta} \lambda_{\theta}}{D} \quad (9)$$

$$T_w = T_b + \frac{q_w}{h_b} \quad (10)$$

Then, Eqs. (8)–(10) are solved iteratively until the convergence of the wall temperature is achieved.

2.1.4. Determination of the critical heat flux for DHT

The empirical correlation proposed by Mokry et al. (2011) to predict the value of the minimum heat flux (q_{dht}) for given mass flux at which DHT occurs is as follows:

$$q_{dht} = -58.97 + 0.745G \quad (11)$$

It means that NHT occurs when $q_w < q_{dht}$ and DHT occurs when $q_w > q_{dht}$.

The above mentioned empirical correlation is based on the mass flux only. Therefore, it does not account for other factors that might affect DHT. Although this is a simplified correlation, it can predict

successfully the occurrence of DHT for the cases under consideration in the present study when comparing with the experimental data. But it cannot predict the deteriorated heat transfer zone (DHTZ).

2.2. Mathematical formulation of the CFD model

In the current CFD simulations, the axi-symmetric assumption is used for the simulation of the fluid flow and heat transfer in circular tubes. The governing equations used for the supercritical water flow in uniformly heated vertical circular tubes are the conservation of mass, momentum and energy. The Reynolds averaged form of these governing equations can be expressed in a tensor form as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho \bar{u}_i) = 0; \quad (12)$$

$$\frac{\partial}{\partial t} (\rho \bar{u}_i) + \frac{\partial}{\partial x_j} (\rho \bar{u}_i \bar{u}_j) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \bar{u}_i}{\partial x_j} - \rho \bar{u}_i' u_j' \right) \quad (13)$$

$$\frac{\partial}{\partial t} (\rho C_p T) + \frac{\partial}{\partial x_i} (\bar{u}_i \rho C_p T) = \frac{\partial}{\partial x_i} \left[\left(k + \frac{C_p \mu_t}{Pr_t} \right) \frac{\partial T}{\partial x_i} \right] + \phi \quad (14)$$

To solve for the Reynolds stress term ($\rho \bar{u}_i' u_j'$), two turbulence models are selected in the current study, RSM and $k-\omega$ SST model. The equation for the transport of the Reynolds stresses in the RSM is presented below (ANSYS Inc.).

$$\begin{aligned} \underbrace{\frac{\partial}{\partial t} (\rho u_i' u_j')}_{\text{Local Time Derivative}} + \underbrace{\frac{\partial}{\partial x_k} (\rho u_k u_i' u_j')}_{C_{ij}=\text{Convection}} = & -\underbrace{\frac{\partial}{\partial x_k} [\rho u_i' u_j' u_k' + p'(\delta_{ik} u_j' + \delta_{jk} u_i')]}_{D_{T,ij}=\text{Turbulent Diffusion}} \\ & + \underbrace{\frac{\partial}{\partial x_k} \left[\mu \frac{\partial}{\partial x_k} (u_i' u_j') \right]}_{D_{L,ij}=\text{Molecular Diffusion}} - \underbrace{\rho \left(u_i' u_k' \frac{\partial u_j}{\partial x_k} + u_j' u_k' \frac{\partial u_i}{\partial x_k} \right)}_{P_{ij}=\text{Stress Production}} \\ & - \underbrace{\rho \beta (g_i u_j' \theta + g_j u_i' \theta)}_{G_{ij}=\text{Buoyancy Production}} + \underbrace{p' \left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right)}_{\phi_{ij}=\text{Pressure Strain}} - \underbrace{2\mu \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k}}_{\epsilon_{ij}=\text{Dissipation}} + \underbrace{S_{user}}_{\text{User Defined Source Term}} \end{aligned} \quad (15)$$

The $k-\omega$ SST model has different form than the RSM where the transport equations for the turbulence kinetic energy (k) and specific dissipation (ω) are employed as opposed to Reynolds stresses. The transport equations for k and ω are as follows (ANSYS Inc.),

$$\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{Pr_k} \right) \frac{\partial k}{\partial x_j} \right] + \tilde{G}_k - Y_k \quad (16)$$

$$\frac{\partial}{\partial t} (\rho \omega) + \frac{\partial}{\partial x_i} (\rho \omega u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{Pr_{\omega}} \right) \frac{\partial \omega}{\partial x_j} \right] + \tilde{G}_{\omega} - Y_{\omega} + D_{\omega} \quad (17)$$

where $\tilde{G}_k$: generation of turbulence kinetic energy; $\tilde{G}_{\omega}$: generation of ω ; Y_k : dissipation of turbulence kinetic energy; Y_{ω} : dissipation of ω ; D_{ω} : cross-diffusion term.

The detailed mathematical modelling of the above mentioned terms can be found in (ANSYS Inc.).

The enhanced wall treatment is used for both turbulence models. The mesh structure near the wall is generated such that non-dimensional wall distance $y^+ < 1$ in the entire computational domain ($y^+ = (u_{\tau} y)/\nu$). The SIMPLEC solution scheme is used and the QUICK is used as an interpolation scheme.

Table 1
Parameters corresponding to HTC correlations

	C	θ	n_1	n_2	n_3	n_4	n_5	n_6	n_7	ϕ
HTCD (Incropera, 2011)	0.023	b	0.80	0.40	0.0	0.0	0.0	0.0	0.0	1.0
HTCJ (Jackson, 2002)	0.0183	b	0.82	0.50	0.0	0.30	0.0	0.0	n_j	1.0
where										
$n_j = 0.4$ for $T_b < T_w < T_{pc}$ and $1.2 T_{pc} < T_b < T_w$										
$n_j = 0.4 + 0.2 \left(\frac{T_w}{T_{pc}} - 1 \right)$ for $T_b < T_{pc} < T_w$										
$n_j = 0.4 + 0.2 \left(\frac{T_w}{T_{pc}} - 1 \right) \left[1 - 5 \left(\frac{T_b}{T_{pc}} - 1 \right) \right]$ for $T_{pc} < T_b < 1.2 T_{pc}$ and $T_b < T_w$										
HTCM (Mokry et al., 2011)	0.0061	b	0.904	0.0	0.684	0.564	0.0	0.0	0.0	1.0
HTCS (Swenson et al., 1965)	0.00459	w	0.923	0.0	0.613	0.231	0.0	0.0	0.0	1.0
HTCW (Watts and Chou, 1982)	0.021	b	0.80	0.0	0.55	0.350	0.0	0.0	0.0	ϕ_w
where										
$\phi_w = 1$ for $Bu^* < 10^{-5}$										
$\phi_w = [1 - 3000 Bu^*]^{0.295}$ for $10^{-5} < Bu^* < 10^{-4}$										
$\phi_w = [7000 Bu^*]^{0.295}$ for $Bu^* > 10^{-4}$										
$Bu^* = \frac{\bar{G} r_b}{Re_b^{2.7} \rho_b^{0.50}}$										
and $\bar{G} r_b = g \left(1 - \frac{\rho_w}{\rho_b} \right) \frac{D^3}{v_b^2}$										

Table 2
Mesh information.

Case #	D (mm)	L (m)	# grids in radial direction	# grids in axial direction
1 (Mokry et al., 2011)	10	4	60	4000
2 (Churkin et al., 2011)	10	4	60	4000
3 (Mokry et al., 2011)	10	4	60	4000
4 (Mokry et al., 2011)	10	4	60	4000
5 (Mokry et al., 2011)	8	4	60	4000
6 (Churkin et al., 2011)	25.4	2.79 ^a	60	2790
7 (Ornatskij et al., 1971)	3	1	40	1000

^a Unheated bottom length: 0.63 m, heated intermediate length: 2 m, unheated top length: 0.16 m.

The grid independence tests are carried out for all the cases to ensure the accuracy of results obtained by CFD simulations. For the axi-symmetric CFD simulations, the uniform rectilinear grid is used with the mesh refinement near the wall. Table 2 gives the information on the number of grid cells used for each simulation case.

3. Results and discussion

For the purpose of validation of the proposed numerical models and to carry out the intended analysis, 7 different steady state experimental cases are selected. The details of the experimental parameters are presented in Table 3. q_{dht} listed in Table 3 is calculated from Eq. (11). The experiments under consideration dealt with supercritical water flowing vertically upwards in bare circular tubes subjected to constant and uniform heat flux in the periphery. The selected experimental data sets have broad range of operating conditions in terms of mass flux, heat flux, inlet temperature and operating pressure. Cases 1–3 represent the situation where no DHT was observed experimentally anywhere in the flow region ($q_w < q_{dht}$). Cases 4–7 represent the situation where DHT was observed experimentally ($q_w > q_{dht}$) under low mass flux (Cases 4–6) and high mass flux (Case 7) conditions.

3.1. Validation of the numerical models at steady state condition

The numerical simulations are carried out using both THRUST and CFD models. The comparison of the local heat transfer coefficients predicted by the THRUST using 5 different HTCs with the experimental data for Case 1 is shown in Fig. 1. It is observed that the HTCD and HTCJ overpredict the heat transfer coefficient drastically in comparison to the experimental results for the 2nd half of the tube. Similar trend is observed for other cases also (not shown in the figure). Thus, those two HTCs are not used in the further study.

The HTCM, HTCS and HTCW are found to be comparable with the experimental results in most of the cases. Thus, they are used in the rest of this study. The wall temperatures of the SCW predicted by the THRUST using 3 different HTCs (HTCM, HTCS and HTCW) and CFD using two different turbulence models (RSM and $k-\omega$ SST) are compared with the experimental data for Cases 1–7, as shown in Figs. 2–8, respectively.

The wall temperatures predicted by the THRUST using the HTCM and HTCW and CFD using the RSM and $k-\omega$ SST are shown in Fig. 2 in comparison with the experimental data for Case 1 where no DHT is observed experimentally. The wall temperature predicted by the THRUST using the HTCS shows fluctuating behaviour when the wall temperature initiates to exceed the pseudo-critical temperature (T_{pc}). Later on, not much deviation from experimental results is observed.

Fig. 1. Comparison of the heat transfer coefficient predicted by the THRUST with the experimental data (Mokry et al., 2011) for Case 1 ($q_w/G = 0.39$).

Table 3

Geometrical and operating parameters of the experiments under consideration.

Case #	D (mm)	L (m)	p (MPa)	T_{in} ($^{\circ}\text{C}$)	G ($\text{kg/m}^2\text{s}$)	q_w (kW/m^2)	q_{dht} (kW/m^2)	Re_{in} ($\times 10^4$)
1 (Mokry et al., 2011)	10	4	24.1	350	1503	590	1061	20.8
2 (Churkin et al., 2011)	10	4	24.0	352	1500	884	1059	21.0
3 (Mokry et al., 2011)	10	4	23.9	350	1000	681	688	13.9
0.8 4 (Mokry et al., 2011)	10	4	24.1	350	203	129	93	2.8
0.8 5 (Mokry et al., 2011)	8	4	24.5	210	595	570	384	3.6
0.8 6 (Churkin et al., 2011)	25.4	2.79 ^a	25	200	380	400	224	6.9
0.8 7 (Ornatskij et al., 1971)	3	1	25.5	120	1500	1810	1058	1.9

^a Unheated bottom length: 0.63 m, heated intermediate length: 2 m, unheated top length: 0.16 m. **Fig. 2.** Comparison of the wall temperatures with the experimental data (Mokry et al., 2011) for Case 1 ($q_w/G = 0.39$). **Fig. 4.** Comparison of the wall temperatures with the experimental data (Mokry et al., 2011) for Case 3 ($q_w/G = 0.68$).

The comparison of the numerical results and experimental data for Cases 2 and 3 are shown in Figs. 3 and 4, respectively. In both cases where no DHT occurs, a very good agreement is observed for all the numerical results compared with the experimental data.

The comparison of the numerical results with the experimental data for Case 4 ($q_w/G = 0.64$) in which DHT occurs is shown in Fig. 5. Two DHT zones are observed in the experiment as shown in Fig. 5, one is in the entrance region whereas another one is towards the end of the tube. The CFD models with the RSM and $k-\omega$ SST are able to predict the wall temperature in the beginning of the first DHT region, but they fail to capture the wall temperature towards the end of the first DHT where the bulk temperature (T_b) is close to T_{pc} . It can be observed that the RSM over predicts and $k-\omega$ SST model under predicts the wall temperature in the entrance region

of the tube. Moreover, the $k-\omega$ SST model gives much higher wall temperature in the axial region $z^* = 0.125-0.375$ ($T_b = 366-380^{\circ}\text{C}$), failing to regain wall temperature quickly after the sharp increase at $z^* = 0.125$ which corresponds to the bulk temperature of 366°C . All the results by the THRUST show a very good agreement with the experimental data for Case 4 as shown in Fig. 5, except at the end of the first DHT zone, where the bulk temperature of SCW is near T_{pc} . None of the models succeed in predicting the sharp increase and decrease in the wall temperature at the end of the first DHT zone. But all models of both THRUST and CFD predict the wall temperatures very well for second DHT zone except for the THRUST using the HTCS.

For the Case 5, the wall temperature from the THRUST based on the HTCM is close to the experimental one even in the DHT zone

Fig. 3. Comparison of the wall temperatures with the experimental data (Churkin et al., 2011) for Case 2 ($q_w/G = 0.59$). **Fig. 5.** Comparison of the wall temperatures with the experimental data (Mokry et al., 2011) for Case 4 ($q_w/G = 0.64$).

Fig. 6. Comparison of the wall temperatures with the experimental data (Mokry et al., 2011) for Case 5 ($q_w/G = 0.96$).

except near the outlet, as shown in Fig. 6. The result by the THRUST based on the HTCS also has trend in-line with the experimental data. But, the wall temperature predicted by the HTCS fluctuates when it is near T_{pc} . The $k-\omega$ SST model gives a close agreement with the experimental data, however, the fluctuation in the wall temperature occurs when the wall temperature is higher than T_{pc} and is propagated till the exit of the tube. The RSM gives a more smooth wall temperature distribution compared to the $k-\omega$ SST model.

The results for Case 6, where DHT was observed experimentally, are shown in Fig. 7. The $k-\omega$ SST model captures the DHT phenomenon, but it is offset by around 0.4 non-dimensional distance in the axial direction. The magnitude of the wall temperature in the DHT region is also under predicted by the $k-\omega$ SST model. The RSM is not able to capture the DHT phenomenon, but it gives a better agreement outside DHT region. All the numerical results by the THRUST show a good agreement with the experimental data outside the DHT region.

In Case 7, where the DHT phenomenon was observed experimentally at a high mass flux condition, there is a sharp increase in the wall temperature predicted by the THRUST using the HTCM as shown in Fig. 8. The predicted DHT by the THRUST with the HTCM occurs earlier in the channel than the experiment and the predicted wall temperature is much higher than the experimental data at the beginning of the DHT region. However, the HTCM

Fig. 8. Comparison of the wall temperatures with the experimental data (Mokry et al., 2011) for Case 7 ($q_w/G = 1.21$).

is able to capture the DHT qualitatively whereas, both HTCS and HTCW based THRUST simulations cannot predict the sudden rise in the wall temperature in the DHT region. The numerical results obtained from the CFD model using the $k-\omega$ SST model follows the experimental data accurately till the axial location where the peak wall temperature occurs. It fails to regain the wall temperature after it reaches the maximum, similar to that in Case 4. The RSM shows an excellent agreement with the experimental data when the wall temperature is lower than T_{pc} and under predicts the wall temperature when it is higher than the T_{pc} . However, near the exit of the tube, the RSM over predicts the wall temperature. It is also found that there are sharp step changes in the wall temperature for the $k-\omega$ SST model whereas the RSM provides more smooth profile for the wall temperature.

The errors between the numerical and experimental values for the wall temperature are given in Table 4. It shows that the errors are very small for the cases without DHT for all the numerical results. For the cases with DHT, the errors are higher, but of acceptable range except for Case 7 when the HTCM is used in the THRUST. From Table 4, it can be seen that the highest average error using different models occurs in Case 7. This might be due to the fact that Case 7 is the only case with DHT at high mass flux, and it is the only DHT case at high mass flux available from the literature. The errors obtained by the CFD results confine to 5.40% and 5.19% for the RSM and $k-\omega$ SST model, respectively, for all the cases. Except for the Case 7, the maximum errors are 4.49%, 7.09% and 4.46% when HTCM, HTCW and HTCS are used in the THRUST, respectively.

In summary, the wall temperatures predicted by the THRUST and CFD for Cases 1–3 and 5 agree well with the experimental data whereas none of the numerical models can capture the sharp increase in the wall temperature where DHT appeared for Cases 4 and 6, but the numerical models are able to provide a good match in the rest of the channel. The highest average error in the numerical results occurs in Case 7, which is 6.44%. For all the NHT cases (Cases 1–3) and DHT cases (Cases 4–6) at low mass flux, the THRUST based on the HTCM provides the lowest average error (1.9%) among all the numerical results obtained at present, whereas the error for the DHT case at the high mass flux (Case 7) is observed to be the lowest when the HTCS is used. In case of CFD simulations, both turbulence models, the RSM and $k-\omega$ SST model, are found to be comparable to each other for all the cases. Therefore, it can be concluded that a good agreement between the numerical results and the experimental data, in general, is obtained; however, the local discrepancies do exist, but generally are confined to a narrow region inside the channel where DHT takes place.

Fig. 7. Comparison of the wall temperatures with the experimental data (Churkin et al., 2011) for Case 6 ($q_w/G = 1.05$).

Table 4
Relative errors between the numerical and experimental results for the wall temperature.

Case #	Relative errors in the wall temperature, $[T_{w num} - T_{w exp}/T_{w exp}]$ (%)											
	RSM		$k-\omega$ SST		HTCM		HTCW		HTCS		Avg	
	MAE	SD	MAE	SD	MAE	SD	MAE	SD	MAE	SD	MAE	SD
1 (Mokry et al., 2011)	0.35	0.40	0.34	0.44	0.46	0.32	0.30	0.37	0.62	0.72	0.41	0.45
2 (Churkin et al., 2011)	0.91	1.03	1.29	1.45	1.67	1.80	1.06	1.14	0.65	0.81	1.12	1.25
3 (Mokry et al., 2011)	1.22	1.06	1.56	0.75	1.66	1.56	1.18	1.32	1.80	1.39	1.48	1.22
0.84 (Mokry et al., 2011)	1.70	2.04	2.39	3.32	1.14	1.44	2.12	1.21	1.33	1.54	1.73	1.91
0.85 (Mokry et al., 2011)	5.40	2.98	3.40	2.85	3.03	3.75	7.09	4.68	3.90	4.30	4.57	3.71
0.86 (Churkin et al., 2011)	4.68	4.97	4.21	5.19	3.45	4.49	3.62	4.44	3.69	4.46	3.93	4.71
0.87 (Ornatskij et al., 1971)	3.51	4.96	3.52	5.14	14.90	8.72	5.40	6.49	4.86	5.55	6.44	6.17
Avg	2.54	2.49	2.39	2.73	3.76	3.16	2.97	2.81	2.41	2.68	2.81	2.77

MAE, mean of absolute error; SD, standard deviation.

3.2. Comparison of the numerical models at the transient condition

The in-depth knowledge of dynamic response is vital for safe and smooth operation of nuclear reactors. The SCWR uses single phase supercritical water as the coolant which has different dynamic response than the BWR due to the difference in their TH behaviour. As an initial step for studying dynamic response, the unsteady heat transfer and flow analysis of supercritical water is investigated in vertical circular tubes. For this purpose, two critical input parameters – mass flow rate and heat flux, are varied with time. In response to those changes, the temporal variation of the outlet mass flow rate, outlet bulk temperature and axial wall temperature are obtained using both THRUST and CFD models. As previously discussed, the heat transfer deterioration phenomenon is critical to the SCWR and hence the DHT needs to be studied under transient conditions. DHT might occur when the mass flow rate decreases while keeping the heat flux unchanged or heat flux increases while keeping the mass flow rate unchanged. In the present study, the transient simulation is started with an initial equilibrium condition where DHT was narrowly missed, but likely to occur during the transient process. Three transient conditions are considered, 2 of them with the step change in the input mass flow rate and wall heat flux, respectively and 1 with a periodic change in the input mass flow rate.

Case 3 is selected for the initial condition of the transient study. It represents a situation where DHT was not observed in the experiment, but is predictably close to the occurrence of the DHT phenomenon in the channel since the heat flux ($q_w = 681 \text{ kW/m}^2$) is very close to the minimum heat flux for DHT to occur ($q_{dht} = 688 \text{ kW/m}^2$) as shown in Table 3. The transient simulations are carried out by the THRUST using the HTCM and CFD using the $k-\omega$ SST model.

The transient results corresponding to the step change in the inlet mass flow rate are shown in Fig. 9. The perturbed value of the inlet mass flow rate is chosen such that the DHT phenomenon is anticipated to occur for the given heat flux. Based on Eq. (11) it is estimated that the DHT phenomenon may occur during this transient process when the mass flux is lower than $993.2 \text{ kg/m}^2 \text{ s}$ at the given heat flux for Case 3. So, the perturbation in the mass flow rate is from $1000 \text{ kg/m}^2 \text{ s}$ to $800 \text{ kg/m}^2 \text{ s}$ (i.e., 20% reduction). The introduction of the perturbation in the input mass flow rate results in initial oscillations of the mass flow rate at the outlet for both the CFD and THRUST simulations as shown in Fig. 9a. However, the oscillations die out subsequently. The outlet mass flow rate decreases with time and finally achieves the asymptomatic steady state value, which is equal to the perturbed inlet mass flow rate holding the continuity for the newly obtained equilibrium condition. The steady state values obtained using the CFD and THRUST approaches are similar. However, the oscillation predicted by the THRUST dies sooner than that predicted by the CFD model and the

(a) Temporal variation of the mass flow rate

(b) Temporal variation of the bulk temperature of the coolant

(c) Axial variation of the wall and bulk temperatures at different time

Fig. 9. Step decrease in the inlet mass flow rate by 20% for Case 3.

flow rate predicted by the THRUST reaches the final steady state about 0.5 s earlier than that by the CFD model. The outlet bulk temperature, as observed in Fig. 9b, also shows the oscillating behaviour in the initial transient period, but the amplitude of oscillations is negligible. DHT can be identified by a sudden increase in the wall temperature as shown in Fig. 9c. It can be seen from Fig. 9c that the wall temperature at the inlet predicted by the CFD is much lower

Table 5

Relative difference obtained by the CFD and THRUST for the wall temperature (%).

Case description	Relative difference in the wall temperature			
	Time = 1 s		Final steady state	
	MAE	SD	MAE	SD
Step change in mass flow rate	2.80	3.18	2.67	3.04
Step change in heat flux	1.51	1.73	1.45	1.69

Case description	Relative difference in the wall temperature			
	Time = 1 s		Time = 2 s	
	MAE	SD	MAE	SD
Sinusoidal change in mass flow rate	0.64	0.82	0.64	0.82

than that from the THRUST model. But, there is a sudden increase in the wall temperature near the inlet predicted by the CFD. So, the difference in the wall temperatures predicted by the two models becomes very small short after the inlet. Consequently, there is an increase in the wall temperature and then a decrease, which corresponds to DHT, as shown in Fig. 9c. Both THRUST and CFD model predict DHT near the inlet of the channel. But, the DHT zone predicted by the THRUST is between $z^* = 0-0.125$ which corresponds to $T_b = 351.5-370^\circ\text{C}$, whereas the CFD model predicts it between $z^* = 0.012-0.262$ where the bulk temperature varies from 370°C to 379°C . In the exit region, the CFD model and THRUST give similar predictions. The difference in the wall temperatures by the CFD model and THRUST at the exit is lower than the entrance region. The difference in the predicted wall temperatures using the THRUST and CFD model is shown in Table 5. Contrary to the wall temperature, the bulk temperature shows excellent agreement between the results obtained by the CFD model and THRUST as shown in Fig. 9b and c. The difference in the predicted wall temperatures might be due to the empiricisms involved in the HTC correlation used in the THRUST.

The transient results corresponding to the step change in the wall heat flux rate are shown in Fig. 10. Based on Eq. (11), $q_{dht} = 688 \text{ kW/m}^2$ for the given mass flux for Case 3. So, the heat flux is changed step wise from 681 kW/m^2 to 749 kW/m^2 (i.e., 10% increase) with an anticipation that the DHT may take place during the transient process. For this transient case study, the mass flux is unchanged and therefore, based on Eq. (11) it is also expected that the minimum value of heat flux, at which DHT may take place, also remains the same. The trend of the outlet mass flow rate, as shown in Fig. 10a, is similar to the case when the step change occurs in the inlet mass flow rate. The final steady state value of the outlet mass flow rate matches exactly with the inlet mass flow rate for both CFD models and THRUST. The outlet bulk temperature, as observed in Fig. 10b, also has similar qualitative trend as the previous case and the initial oscillations are predicted by both CFD model and THRUST. The amplitude and time span of the oscillations are always higher in the CFD results compared to the THRUST results. The axial variations of the wall temperature and bulk temperature at different time are shown in Fig. 10c. The comparison of the bulk temperatures using the CFD model and THRUST, as given in Fig. 10b and c, shows an excellent agreement with each other. Fig. 10c shows that the wall temperature predicted by the CFD model is also much lower than that by the THRUST at the inlet of the channel and there is a sudden increase in the wall temperature predicted by the CFD near the inlet, similar to the previous case shown in Fig. 9c. There is a monotonic increase in the wall temperature predicted by the CFD model along the axial direction of the channel. One also can observe from Fig. 10c that the THRUST predicts DHT at $z^* = 0.175$, but DHT is not predicted by the CFD model for the entire channel.

The wall temperature predicted by the CFD model and THRUST are very close at the outlet.

Next, the transient simulations are carried out for the case where inlet mass flux is varied sinusoidally with time. The amplitude of the oscillating inlet mass flux is set to be 20% of the initial value of

(a) Temporal variation of the mass flow rate

(b) Temporal variation of the bulk temperature of coolant

(c) Axial variation of the wall and bulk temperatures at different time

Fig. 10. Step increase in the wall heat flux by 10% for Case 3.

(a) Temporal variation of the mass flow rate

(b) Temporal variation of the bulk temperature of coolant

(c) Axial variation of the wall and bulk temperatures at different time

Fig. 11. Sinusoidal variation of the inlet mass flow rate for Case 3.

1000 kg/m² s to ensure that the mass flux in the channel remains lower than the critical value, 993.2 kg/m² s, at the given heat flux condition for a considerable portion of the time period and therefore, the DHT phenomenon occurs in the channel within that time period. The resultant transient response can be seen in Fig. 11. After the initial oscillations, the outlet mass flow rate and bulk temperature, as observed in Fig. 11a and b, respectively, take about 1.5 s to get to the periodic steady state, after which both show periodic trend similar to the inlet mass flow rate. The axial variations of the wall and bulk temperatures at different times are shown in Fig. 11c. A very good agreement between the results obtained by the THRUST and CFD model is observed. The DHT zone predicted by both models almost coincides to each other. Table 5 also confirms the good agreement among the numerical results from the two models.

4. Conclusions

In this paper, an in-house 1-D numerical code, THRUST, and CFD models are validated with the experimental data for the SCW flow in circular tubes. Both models are first used to predict the wall temperature at different operating conditions when the channels

are subjected to imposed wall heat flux BC. The wall temperatures obtained from both the numerical models are compared with each other and with the experimental data to verify the models and to identify their limitations. The comparisons indicate that the results for both THRUST and CFD agree well with the experimental data for the cases of NHT where the maximum error is consistently below 2%.

The predicted wall temperatures for the cases of DHT have higher error than the NHT cases. For the two turbulence models examined, none of them is found to be unanimously better than the other for all the cases. However, the RSM provides more smooth wall temperature profiles compared to the $k-\omega$ SST model. The $k-\omega$ SST model fails to retrieve the wall temperature values in some DHT cases that results in conservative estimate in the wall temperature. Similarly, for the THRUST, no single heat transfer correlation is found to be the best for all the cases, however, the HTCW, HTCW and HTCS in general provide satisfactory results. For the case of DHT with a low mass flux and high mass flux, the maximum errors associated with both the RSM and $k-\omega$ SST model are within 5.4% and 5.19%, respectively. For the THRUST, the maximum errors associated with the HTCW, HTCW and HTCS are 4.5%, 7% and 4.5%, respectively, for NHT and DHT with a low mass flux condition. For the case of DHT with a high mass flux condition, the THRUST with the HTCW provides a maximum error about 15% whereas the HTCW and HTCS provide a maximum errors of 6.5% and 5.6%, respectively. It is also found that for the case of DHT with a high mass flux, the $k-\omega$ SST model gives oscillating profiles for the wall temperature.

After satisfactory validation of the THRUST and CFD models with 7 different experimental cases of steady state heat transfer, transient simulations under 3 conditions are carried out. Out of these 3 conditions, 2 of them involve the step change in the input mass flow rate and heat flux whereas third one is of a sinusoidal variation in the input mass flow rate. The THRUST and CFD models are able predict the temporal and axial variations of the wall and bulk temperatures, and the predictions by the THRUST and CFD models are in a good agreement. The temporal variation of the outlet mass flow rate and outlet bulk temperature for all the cases obtained by the THRUST and CFD model show the exact value at the final steady state, but the actual time taken to reach to the final steady state is more in the case of the CFD model than the THRUST. The comparative analysis shows that the THRUST and CFD models are capable to simulate the transient TH behaviour for the SCW flow and heat transfer and therefore, both the numerical models can further be extended and used in the future for the analysis of various dynamic case studies.

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