A Numerical Thermal-Hydraulic Model to Simulate the Fast Transients in a Supercritical Water Channel Subjected to Sharp Pressure Variations

Goutam Dutta1,*,†, Jin Jiang2, Rohit Maitri3 and Chao Zhang3

1 Mechanical Engineering, PDPM Indian Institute of Information Technology, Design and Manufacturing Jabalpur, Jabalpur: 482 005, Madhya Pradesh, India; Electrical and Computer Engineering, University of Western Ontario (UWO), London, Ontario, N6A 5B9, Canada.

2 Electrical and Computer Engineering, University of Western Ontario (UWO), London, Ontario, N6A 5B9, Canada.

3 Mechanical and Materials Engineering, University of Western Ontario (UWO), London, Ontario, N6A 5B9, Canada.

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Abstract. The present work demonstrates the extension of a thermal-hydraulic model, THRUST, with an objective to simulate the fast transient flow dynamics in a supercritical water channel of circular cross section. THRUST is a 1-D model which solves the nonlinearly coupled mass, axial momentum and energy conservation equations in time domain based on a characteristics-dependent fully implicit finite difference scheme using an Eulerian approach. The model developed accounts for the compressibility of the supercritical flow by considering the finite value of acoustic speed in the solution algorithm and treats the boundary conditions naturally. A supercritical water channel of circular cross section, for which the experimental data is available at steady state operating conditions, is chosen for the transient simulations to start with. Two different case studies are undertaken with a purpose to assess the capability of the model to analyze the fast transient processes caused by the large reduction in system pressure. The first transient case study is where the initial exit pressure is reduced by 1 MPa exponentially in a time span of 5 s. In the second case study, the transient is initiated with a sudden step decrease in the exit pressure by the same amount. Results obtained for both the case studies show the desired performance from the model developed.

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Key words: Thermal-hydraulic model, supercritical water, fast transients due to large reduction in system pressure.

*Corresponding author. Email addresses: gd@iiitdmj.ac.in (G. Dutta), jjiang@eng.uwo.ca (J. Jiang), rmaitri@uwo.ca (R. Maitri), czhang@eng.uwo.ca (C. Zhang)

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1 Introduction

The study of supercritical water, though has been carried out extensively through many research works, primarily the experimental ones [1,2], in last several decades, poses many challenges still to-date. The prediction of thermal-hydraulic (TH) behavior on the occasion of fast transient processes is one of such issues. Moreover, the related study has generated a renewed interest at present in the scientific community. The worldwide effort to develop a supercritical water reactor (SCWR), which potentially can provide the improved thermal efficiency at a reduced price and lower maintenance, has triggered the inspiring motivation to the researchers. The various numerical research works [3, 4] carried out recently confirm that the sharp variation of thermo-physical properties of supercritical fluid (SCF) close to the pseudo-critical point (PCP) is an important factor which makes the predictive assessment more difficult. Therefore, it is natural to expect that the significant change in TH behavior of supercritical water (SCW) may take place in the event of transients initiated due to large change in system pressure. It is to be noticed that the fast transient process caused by the large reduction in system pressure is a common phenomenon in case of loss of coolant accident (LOCA) scenario likely to occur due to pump failure or leakage in the piping system of a SCWR plant. On the other hand, the available literature shows that there are numerous research works related to SCF which mainly confined to steady state analysis and investigation of density wave instability [5,6] in SCWR channels where neither the fast transient process took place nor it was caused due to large change in system pressure. However, fast transient depressurizing events have recently been studied experimentally [7] and numerically [8,9] for another supercritical fluid, CO$_2$, used for the application of carbon capture and storage, different from the SCWR technology. The studies were carried out to analyze the effect of leakage of supercritical CO$_2$ into the ambient air in the event of an accidental crack in a pipe line caused during its transportation.

The present investigation is carried out with the objective to analyze the TH behavior of SCW, flowing in a vertically upward circular tube, in the event of transients caused by large reduction in system pressure with the help of an in-house transient Thermal-Hydraulic solver Undertaking Supercritical waTer (THRUST). THRUST has already been validated [10,11] by comparing the results with the available experimental data, and with the Fluent based CFD results and the available numerical results. Two case studies are undertaken, one where transient is initiated due to gradual, but large decrease of the exit pressure by 1MPa and for the other one, there is sudden step decrease in the exit pressure by the same amount.

2 Numerical model development

THRUST is a 1-D model developed to take into account the variation of field variables in the axial direction.
2.1 Transient solution

The model solves the following nonlinearly coupled mass, momentum and energy conservation equations in the time-domain:

\[
\frac{\partial}{\partial t} \begin{bmatrix} \mathbf{R} \\ \mathbf{S} \end{bmatrix} + \frac{\partial}{\partial z} \begin{bmatrix} \mathbf{S} \end{bmatrix} = \begin{bmatrix} \mathbf{T} \end{bmatrix},
\]  

(2.1)

where

\[
\mathbf{R} = \begin{bmatrix} \rho A \\ \rho A u \\ \rho A e \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} \rho A u \\ A (pu^2 + p) \\ \rho A u e_f \end{bmatrix},
\]

\[
\mathbf{T} = \begin{bmatrix} p \frac{dA}{dz} - \tau_w P_w - \rho A \delta \frac{dH}{dz} - \frac{1}{2} \sum_{i=1}^{n} \delta(z - z_i) \rho_i u_i^2 \\ q_w' p_H \end{bmatrix},
\]

and \( e = e_f - \frac{p}{\rho} \) and \( e_f = h + \frac{u^2}{2} + gH \).

In addition to the conservation equations, the equation of state, \( \rho = \rho(p, h) \), is used with the help of a NIST steam routine to account for the pressure and enthalpy dependent variation of thermodynamic properties along the axial direction of the tube.

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

\[
\frac{\partial}{\partial t} \begin{bmatrix} \mathbf{U} \end{bmatrix} + \mathbf{A} (\mathbf{U}) \frac{\partial}{\partial z} \begin{bmatrix} \mathbf{U} \end{bmatrix} = \begin{bmatrix} \mathbf{D} (\mathbf{U}) \end{bmatrix},
\]

(2.2)

where \( \mathbf{U} \) is a vector of unknown dependent variables \( [W, h, p]^T \), and \( \mathbf{A} \), a square coefficient matrix and \( \mathbf{D} \), a source vector, are functions of \( \mathbf{U} \).

The eigenvalues of the coefficient matrix \( \mathbf{A} \) are next obtained and found to be real \( (u, u+a, u-a) \). Hence the PDEs, Eq. (2.2) which can be classified as hyperbolic equations are next transformed into a characteristic form as the following:

\[
\frac{\partial}{\partial t} \begin{bmatrix} \mathbf{U} \end{bmatrix} + \overline{\mathbf{A}} \frac{\partial}{\partial z} \begin{bmatrix} \mathbf{U} \end{bmatrix} = \begin{bmatrix} \mathbf{C} \end{bmatrix},
\]

(2.3)

where \( \overline{\mathbf{A}} \) is a diagonal matrix of eigenvalues of \( \mathbf{A} \).

The model discretizes the convective terms of Eq. (2.3) with the help of a characteristics-dependent implicit finite difference scheme using a fixed spatial and temporal grid distribution, i.e., in an Eulerian frame of reference. The finite value of the acoustic speed \( (a \equiv \sqrt{\frac{\partial p}{\partial \rho}}) \) is first obtained with the help of the equation of state and then used in the mathematical formations and thereby, allows the model to account for the compressibility of SCW. The solution algorithm employed in the model treats the boundary conditions (BCs) naturally without the use of any shooting method.
The PDEs in Eq. (2.3) can be expressed into the Lagrangian frame of reference and can further be transformed into the ordinary differential equations (ODEs) which will be compatible along the respective characteristic directions. These compatible ODEs can be solved into their respective characteristic directions. A detailed mathematical analysis carried out earlier by Dutta and Doshi [12] demonstrated that for the present and similar subsonic flow situations \((u < a)\), one can specify either pressure and enthalpy, or enthalpy and mass flow rate (or velocity), but one can’t specify pressure and mass flow rate (or velocity) together as inflow BCs; whereas any one among pressure, enthalpy, mass flow rate (or velocity) can be specified as outflow BC. The transient simulations carried out in the present investigation correspond to the case studies where the enthalpy and mass flow rate are specified at the inlet and the pressure is specified at the exit.

THRUST, which was earlier used to analyze behaviour of SCW flowing vertically upwards in a circular channel [10] and to simulate density wave dynamic instabilities for the CANDU SCWR [11] considering single and parallel channels in the reactor core, because of its capability to account for the compressibility of SCW is at present extended to capture fast transients caused by large reduction in the system pressure.

### 2.2 Steady state solution

The resultant discretized equations for steady state flows are as follows:

\[
\rho_{i+1} A_{i+1} u_{i+1} = \rho_i A_i u_i, \quad (2.4a)
\]

\[
p_i - p_{i+1} = \frac{1}{2} \left( \frac{1}{A_i} + \frac{1}{A_{i+1}} \right) \left[ \left( \rho A u^2 \right)_{i+1} - \left( \rho A u^2 \right)_i \right] + \frac{1}{2} \left( \rho (F + g) \right)_i + \left( \rho (F + g) \right)_{i+1} (z_{i+1} - z_i), \quad (2.4b)
\]

\[
(e_f)_{i+1} - (e_f)_i = \frac{1}{2} \left[ \left( \frac{q'_w}{\rho A u} \right)_i + \left( \frac{q'_w}{\rho A u} \right)_{i+1} \right] (z_{i+1} - z_i). \quad (2.4c)
\]

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 field variables, i.e., the velocity (or mass flow rate), enthalpy and pressure at the inlet are specified, otherwise a shooting method along with the forward marching scheme is employed.

### 2.3 Heat transfer coefficients

The wall temperature is determined from THRUST using three different heat transfer coefficient (HTC) correlations provided by Mokry et al. [13] (HTCM), Swenson et al. [1] (HTCS) and Watts et al. [14] (HTCW). The above mentioned HTC correlations have the following general form:

\[
Nu_{th} = C \times Re_{th}^{n_1} Pr_{th}^{n_2} Pr_{\infty}^{n_3} \left( \frac{\rho w}{\rho \infty} \right)^{n_4} \left( \frac{\mu w}{\mu \infty} \right)^{n_5} \left( \frac{k w}{k \infty} \right)^{n_6} \left( \frac{\tau_p}{c_{\infty}} \right)^{n_7} \phi, \quad (2.5)
\]
where $\phi \equiv \phi\{z,T_\infty,T_w,\cdots\}$ and the subscript, $\theta$, may be $\infty$, $w$ or $f$ depending on whether the bulk temperature, $T_\infty$, wall temperature, $T_w$ or mean film temperature, $T_f = \frac{1}{2}(T_\infty + T_w)$ is used in the corresponding correlation. The parametric details of these 3 HTCs are listed in the Table 1.

Table 1: Parameters corresponding to HTC correlations.

<table>
<thead>
<tr>
<th>Item</th>
<th>C</th>
<th>$\theta$</th>
<th>$n_1$</th>
<th>$n_2$</th>
<th>$n_3$</th>
<th>$n_4$</th>
<th>$n_5$</th>
<th>$n_6$</th>
<th>$n_7$</th>
<th>$\phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HTCM [13]</td>
<td>0.0061</td>
<td>$\infty$</td>
<td>0.904</td>
<td>0.0</td>
<td>0.684</td>
<td>0.564</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>HTCS [1]</td>
<td>0.00459</td>
<td>$w$</td>
<td>0.923</td>
<td>0.0</td>
<td>0.613</td>
<td>0.231</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>HTCW [14]</td>
<td>0.021</td>
<td>$\infty$</td>
<td>0.80</td>
<td>0.0</td>
<td>0.55</td>
<td>0.350</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>$\phi_w$</td>
</tr>
</tbody>
</table>

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 $Bu^* > 10^{-4}$

$Bu^* = \frac{Gr_\infty}{Re_\infty^{2/3} Pr_\infty^{1/3}}$

and $Gr_\infty = g \left(1 - \frac{\rho_w}{\rho_\infty}\right) \frac{D^3}{\nu_\infty^2}$

### 2.4 Determination of the local wall temperature

All the field variable representing the bulk properties of the SCW are first obtained and then, the wall temperature is determined using the present methodology. To initiate the procedure, the wall temperature is assumed first and then, the heat transfer coefficient, $h_\infty$, is obtained by using Eq. (2.6) and one of the HTCM, HTCS and HTCW obtained from Eq. (2.5)

$$h_\infty = \frac{Nu_{\theta} k_d}{D}. \quad (2.6)$$

The wall temperature, $T_w$, is next updated using the following Eq. (2.7):

$$T_w = T_\infty + \frac{q_w}{h_\infty}. \quad (2.7)$$

Next, Eqs. (2.5)-(2.7) are solved iteratively until the convergence in the wall temperature is achieved.

### 2.5 Grid independent tests and validation

To obtain the grid independent results, several simulations are performed with different number of nodes which are equally-spaced and different time step sizes. It is found that the results obtained from THRUST turn out to be independent with spatial and temporal
grid sizes when the axial length of the circular channel is divided into 100 mesh points and for the transient simulations, a time step size of 0.001 s is chosen. Therefore, the further simulations are carried out with the grid distribution as mentioned above.

The capability of THRUST to analyze the behavior of supercritical flow in a circular channel has already been validated in an earlier research work by Dutta et al. [10]. The results obtained from THRUST agreed reasonably well with the available experimental data and from that obtained by Fluent based CFD results. The capability of THRUST to simulate the dynamic density wave instability in a supercritical water channel has also been validated by Dutta et al. [11].

3 Results and discussion

The present investigation is carried out for a case where the SCW is flowing in a circular channel and the experimental data [13] is available for the channel when operating at the steady state conditions.

3.1 Steady state results

The experiment under consideration dealt with supercritical pressure water flowing vertically upwards in a circular tube subjected to constant and uniform heat flux at the periphery of the circular tube. The geometrical dimensions of the tube and its steady state operating conditions are listed in Table 2. The comparison of the steady state results obtained from THRUST and that from experimental data is shown in Fig. 1. The results indicate a reasonably good agreement between the numerical prediction from THRUST and the available experimental data. For the HTCM, the error in the wall temperature between that obtained with the HTCM and experimental data is maximum (10 %) at the inlet of the channel and it gradually decreases with the increase of the axial length. A good agreement in wall temperature is obtained for the axial length between $z = 1 - 3.5 \text{ m}$ and for the rest of channel, $z = 3.5 - 4.0 \text{ m}$, the maximum deviation is limited to 4 %. It

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Diameter, D (mm)</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Length, L (m)</td>
<td>4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Initial steady state operating conditions</th>
<th>Mass flux, $G$ (kg/m$^2$s)</th>
<th>1000</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Inlet temperature, $T_{in}$ (°C)</td>
<td>350</td>
</tr>
<tr>
<td></td>
<td>Inlet pressure, $p_{in}$ (MPa)</td>
<td>23.9</td>
</tr>
<tr>
<td></td>
<td>Heat flux, $q$ (kW/m$^2$)</td>
<td>681</td>
</tr>
</tbody>
</table>
### Figure 1: Comparison of the wall temperature obtained from THRUST with the experimental data at initial steady state operating conditions [10, 13].

is also observed that the maximum error of 10% happens to be at the location where the wall temperature in the experimental data reaches the pseudo critical point where sharp variation in the thermophysical properties takes place and therefore, the evaluation of property of the wall and the adjacent coolant is expected to be uncertain. In case of the HTCS, the obtained wall temperature agrees well with the experimental data when $z = 0 - 1.35$ m. For the wall temperature obtained with the HTCW, a good agreement is obtained when $z = 0 - 0.7$ m and $z = 2.5 - 3.5$ m. The results, in overall sense, therefore indicate that the wall temperature obtained with all the HTC correlations under consideration provide, more or less, satisfactory agreement with the experimental data. The intended transient analysis will next be carried out using the HTCM.

## 3.2 Transient results

The intended transient simulations are carried out for the SCW flow in the circular tube, described in Section 3.1, when subjected to sharp pressure variations. The steady state results obtained act as the initial condition for the transient simulation. The transient is initiated by perturbing the exit pressure from its initial steady state value while keeping other BCs the same, i.e., for the same enthalpy and mass flux at the inlet of the tube. The first transient case study #1 corresponds to large and fast reduction of the exit pressure by $1 MPa$ exponentially within a span of 5s time, whereas the second transient case study #2 represents instantaneous step reduction in exit pressure by the same amount. The BCs used for the transient simulations are listed in Table 3. Both these case studies are undertaken in order to evaluate the capability of THRUST to simulate the fast transient processes caused by large reduction in the exit pressure. The relevant results for the cases #1 and #2 are shown in Figs. 2 and 3 respectively.
Table 3: Transient operating parameters.

<table>
<thead>
<tr>
<th>Case study</th>
<th>#1</th>
<th>#2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary conditions</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Constant inlet mass flux, $G_{in}$</td>
<td>$G_{in}(t=0)$</td>
<td></td>
</tr>
<tr>
<td>Constant inlet enthalpy, $h_{in}(t)$</td>
<td>$h_{in}(t=0)$</td>
<td></td>
</tr>
<tr>
<td>Pressure drop at exit, $\Delta p_{ex}$ (MPa)</td>
<td>$1 - \exp(-t)$</td>
<td>1.0</td>
</tr>
<tr>
<td>where $\Delta p_{ex} = (p_{ex}(t=0) - p_{ex}(t))$</td>
<td>$1 - \exp(-5)$</td>
<td></td>
</tr>
</tbody>
</table>

3.3 Case study #1: Transient due to exponential decrease in the exit pressure

For the case study #1, the time dependent responses of the mass flow rate and bulk specific enthalpy of the SCW at the exit of the tube are observed in Figs. 2(a) and 2(b) respectively. The temporal variation of the bulk pressure of the SCW at the inlet of the tube is observed in Fig. 2(c). Fig. 2(d) describes the time dependent behavior of the bulk coolant temperature at both the inlet and exit of the tube. In all these Figs. 2(a)-2(d), the initial oscillations of the dependent field variables, which get initiated following the perturbation in the system, are found to be gradually dying down with time and finally reaches to the new asymptotic steady state condition. The mass flow rate at the exit, as observed in Fig. 2(a), undergoes oscillations initially. Later on, the magnitude of the exit mass flow rate is found to be approaching the magnitude of the inlet mass flow rate asymptotically and finally, at the end of 6s, the difference between the exit and inlet mass flow rate ceases to exist; and therefore, it confirms the final attainment of the new steady state condition. Fig. 2(e) shows the axial distribution of mass flow rate at different time. The sharp axial variation of mass flow rate is found to be gradually disappearing as the time advances and it becomes uniform at 8s which reconfirms the establishment of the new asymptotic steady state condition. The axial variation of temperature of the coolant and wall at different time are observed in Fig. 2(f) which indicates that difference between the axial temperature profiles of the coolant at different time gradually reduces with the progress of time and the similar trend is observed for the axial profiles of the wall temperature as well.

3.4 Case study #2: Transient due to step decrease in the exit pressure

For the case study #2, the time dependent responses of the various field variables are shown in Figs. 3(a)-3(d). The results indicate the similar behavior of the field variables as observed in the previous case study, but the new asymptotic steady state condition at the present case is attained at time 2s. The faster attainment of the new asymptotic steady state condition in the present case study in comparison to the previous case study is because of the instantaneous step decrease of the exit pressure here, whereas the pressure at the exit in the previous case study was reduced by the same amount exponentially.
in a span of 5 s time. In addition, more pronounced oscillations because of the stepwise reduction in the exit pressure, following the introduction of the perturbation, with higher amplitude are observed in the present case.
4 Conclusions

The present work demonstrates the development of a numerical model (THRUST) which can simulate TH behavior of SCW in steady as well as unsteady operating conditions. THRUST is a 1-D model based on an efficient solution algorithm which accounts for the compressible flow of SCW and treats the BCs naturally without the use of any shooting method. Three HTC correlations, HTCM, HTCS and HTCW, are used in THRUST to determine the wall temperature for imposed wall heat flux BC. The profile of axial wall temperature at steady state obtained from THRUST is compared with the available experimental data and the comparison shows a good agreement. It is to be noticed that the capability of THRUST to simulate the transients can not be verified because of the lack of experimental data considering the existing state of the art and therefore, one has to rely on numerical predictions. It is also worth to notice that it has already been verified in an earlier research work where the results obtained from THRUST for various transient case studies agreed well that obtained from Fluent based CFD results.
In the present research work, two transient case studies are undertaken in order to evaluate the capability of the model to simulate fast transient processes caused by the large reduction in the exit pressure. The first transient case study deals with gradual reduction in the exit pressure with time and the second one corresponds to the instantaneous decrease in the exit pressure. In both the case studies, the results obtained from THRUST are in expected line and consistent and therefore, the predictions from THRUST are considered to be sufficiently satisfactory. Therefore, the results obtained for both the case studies indicate the potential of THRUST to analyze the fast transient cases in the event of loss of coolant accidents in a SCWR plant where a large reduction in the system pressure is expected in a short span of time.

Acknowledgments

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Nomenclature

\begin{itemize}
  \item \( A \) Area, \( m^2 \)
  \item \( a \) Acoustic speed, \( m/\text{s} \)
  \item \( c_p \) Specific heat capacity at constant pressure, \( J/kgK \)
  \item \( \overline{c_p} \) \( (h_\infty - h_w) / (T_w - T_\infty) \), \( J/kgK \)
  \item \( D \) Diameter of a tube, \( m \)
  \item \( e \) Specific total internal energy, \( J/kg \)
  \item \( e_f \) Specific total flow energy, \( J/kg \)
  \item \( g \) Gravitational acceleration, \( m/s^2 \)
  \item \( G \) Mass flux, \( kg/m^2s \)
  \item \( h \) Specific enthalpy, \( J/kg \)
  \item \( h_\infty \) Heat transfer coefficient, \( W/m^2^\circ C \)
  \item \( k \) Thermal conductivity, \( W/mK \)
  \item \( p \) Pressure, \( Pa \)
  \item \( q \) Heat flux, \( W/m^2 \)
  \item \( q''_w \) Wall heat power per unit area, \( W/m^2 \)
  \item \( q'_w \) Wall heat power per unit length, \( W/m \)
  \item \( t \) Time, \( s \)
  \item \( T \) Temperature, \( ^\circ C \)
  \item \( T_\infty \) Bulk Temperature, \( ^\circ C \)
  \item \( s \) Specific entropy, \( J/kgK \)
  \item \( u \) Velocity, \( m/s \)
  \item \( z \) Axial Location, \( m \)
\end{itemize}
Greek Letters

\( \mu \) Dynamic viscosity, \( \text{Pas} \)
\( \nu \) Kinematic viscosity, \( \text{m}^2/\text{s} \)
\( \rho \) Density of a fluid, \( \text{kg/m}^3 \)
\( \tau_w \) Wall shear stress, \( \text{N/m}^2 \)

Subscripts

ex Exit
in Inlet
\( \infty \) Bulk
pc Pseudo-critical
w Wall

Dimensionless Numbers

\( Bu^* \) Buoyancy Parameter, \( \sqrt[2.7]{Pr_{\infty}^{0.50}} \)
\( Gr_{\infty} \) \( g(1 - \rho_w/\rho_{\infty})D^3/v_{\infty}^2 \)
\( Nu \) Nusselt Number
\( Pr \) Prandtl Number, \( \mu_c p/k \)
\( Pr \) \( \mu c_p/k \)
\( Re \) Reynolds Number, \( \rho u D/\mu \)

Acronyms

BC Boundary condition
HTC Heat transfer coefficient
HTCM Heat transfer coefficient by Mokry et al.
HTCS Heat transfer coefficient by Swenson et al.
HTCW Heat transfer coefficient by Watts et al.
LOCA Loss of coolant accident
PCP Pseudo critical point
SCF Supercritical fluid
SCW Supercritical water
SCWR Supercritical water cooled reactor
TH Thermal-hydraulic
THRUST Thermal-Hydraulic solveR Undertaking Supercritical waTer
References


