Application Of Hlwp Supercritical Light Water Properties In CATHENA

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Abstract

The HLWP (Heavy and Light Water Properties) library provides a computationally efficient means to accurately produce the thermodynamic and thermophysical properties of heavy and light water and the gas properties of air, nitrogen, helium, argon, hydrogen, and carbon dioxide. The light water routines have been updated to provide properties at supercritical pressures for the design of potential future generations of CANDU reactors. The HLWP routines are currently included in a variety of thermalhydraulic programs (CATHENA, ASSERT, TUBRUPT-IST, TEP), and are being considered for inclusion in others (GOTHIC, NUCIRC). The current work describes the accuracy and limitations of the newly developed supercritical routines. Sample results are presented to demonstrate their use in thermalhydraulic calculations and a prototype version of CATHENA.

1. Introduction

The HLWP routines [1] were originally developed by Atomic Energy of Canada (AECL) in the late 1980's to provide thermodynamic and thermophysical properties of heavy (D_2O) and light (H_2O) water for the two-fluid thermalhydraulic code CATHENA [2]. With time, HLWP was also included in a variety of other thermalhydraulic programs (ASSERT, TUBRUPT-IST, TEP), and is being considered for inclusion in others (GOTHIC, NUCIRC). Given this development, it was decided to maintain the HLWP routines as a separate library, and also include all noncondensable property routines used in CATHENA into the library for general use. As a result, the present version of the HLWP library uses a variety of fitted functions to provide a library of routines capable of calculating the thermodynamic and thermophysical properties of heavy and light water and their derivatives as well as the properties of the noncondensable gases air, nitrogen, helium, argon, hydrogen, and carbon dioxide. The purpose of the HLWP library routines is to provide these quantities, on demand from a calling program, in the most efficient, thermodynamically consistent, and accurate manner possible. The routines have been programmed in standard FORTRAN-77 in a manner that allows them to be incorporated into a program running on virtually any operating system.

The original version of HLWP installed in all versions of CATHENA (3.5d/Rev 2 and all previous versions) and all other programs currently making use of HLWP (TUBRUPT, ASSERT, TEP) are referred to HLWP-0.0 or HLWP-0.1. These routines include only the thermodynamic and thermophysical properties of heavy and light water and are described in reference [1]. The current version of HLWP is given the version name HLWP-1.0. The purpose of this paper is to highlight the changes made to the original routines when the HLWP-1.0 version library was assembled. In particular, the re-fitting of the thermodynamic and thermophysical light water properties routines in the subcritical pressure range and the extension of these routines into the supercritical pressure range are discussed in detail.

2. Background

The original HLWP-0.0 and HLWP-0.1 routines provide the properties of light and heavy water only in the subcritical region. Proposed advanced versions of the CANDU reactor could operate in the supercritical pressure region using light water as a primary circuit cooling fluid. As a result, it was felt necessary to extend the HLWP light water properties into the supercritical pressure region. To improve the overall accuracy of the light water routines, make use of the latest available property standards available, and ensure the smooth transition from the subcritical to the supercritical pressure region, it was decided to re-fit both the sub and supercritical pressure properties for light water. The HLWP library uses piecewise Hermite polynomials to represent the thermodynamic property data for heavy and light water as well as their derivatives. The coefficients of the polynomials are obtained by curve fitting the thermodynamic properties to the latest available water property standards. It also uses standard fitted functions to represent the thermophysical properties. The manner in which these fits are obtained is described below.

3. Source of Thermodynamic Properties

Currently, there are two internationally accepted analytical formulations for the thermodynamic properties of light water through formulations defined by International Association for the Properties of Water and Steam (IAPWS):

1. The IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use [3], and
2. The IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam [4].

The 1997 formulation is a re-implementation of the 1995 formulation in which a slight loss of accuracy is traded off in favour of the computational efficiency of the formulation. Since accuracy, smoothness, and consistency of the source are important in the fitting procedure used to create the HLWP-1.0 routines, the 1995 formulation was chosen for use.

The 1995 formulation has two implementations in FORTRAN, one by NIST (the National Institute of Standards and Technology in the USA) and the other by the Lehrstuhl für Thermodynamic, Fakultät für Maschinenbau at the Ruhr-Universität Bochum in Germany. Both implementations were acquired and tested. The test results showed that although the Bochum implementation had some isolated convergence problems and was somewhat slower than the NIST implementation, it was numerically more accurate than the NIST implementation. For this reason, the Bochum routines were chosen as the basis for the fitting functions within the HLWP library.

The generating functions used by the IAPWS standards are not expressed in terms of the dependent variables used by the CATHENA code. They are expressed in terms of Gibbs free energy as functions of density, ρ, and temperature, T,

$$f = f(\rho, T) \tag{1}$$

where f is any thermodynamic property.

In CATHENA, the thermodynamic properties of light and heavy water are required as functions of pressure, P, and enthalpy h,

$$f = f(P,h) \tag{2}$$

The IAPWS generating functions are computationally complex [3]. These functions also require an iteration process to calculate the properties and their derivatives in the form of Equation 3. As a result, the direct use of generating functions would be too computationally inefficient for use in a thermalhydraulic code.

The objective of the HLWP library is to provide a computationally efficient method of determining the thermodynamic properties and their derivatives as functions of pressure and enthalpy required for use in thermalhydraulics codes. It meets this requirement, by re-fitting the official property standards using a piecewise Hermite polynomial approximation. A linear interpolation would be computationally more efficient, but would not be differentiable.

4. Piecewise Hermite Polynomial Approximation

The principle of piecewise approximation is to divide the region in which an approximation is required into several subregions, and to fit (possibly different) functions in each subregion. For the application described here, the fitting functions and their derivatives must be continuous at the boundaries of the subregions. The choice of how to subdivide the original region is of great importance in piecewise approximation. Suppose that not only values but also their derivatives are tabulated at interpolation locations (nodes). This allows:

1) The interpolation polynomial values at these nodes are equal to the tabulated data, and
2) The polynomial derivatives at these nodes also are equal to the tabulated data.

This type of interpolation is called Hermite interpolation.

5. Calculation of Thermodynamic Properties

To maintain mathematical consistency between the thermodynamic properties and their derivatives, the single-state dependent property of specific entropy (s) as a function of absolute pressure (P) and specific enthalpy (h) was chosen for fitting via piecewise Hermite polynomials. All the required properties can then be obtained from the first and second derivatives of specific entropy. These thermodynamic property expressions can be derived from the fundamental relations for an open system under steady state flow condition [4]:

$$du = T\,ds - P\,dv \tag{3}$$

Since specific enthalpy is defined as

$$h = u + Pv \tag{4}$$

differentiating this expression results in

$$dh = du + P\,dv + v\,dP \tag{5}$$

This can be substituted into (3) to form

$$dh = T\,ds + v\,dP \tag{6}$$

or, rearranging,

$$ds = \frac{1}{T}dh - \frac{v}{T}dP \tag{7}$$

From Equation 7, the first order partial derivatives of s are

$$\left.\frac{\partial s}{\partial h}\right|_P \equiv s_h = \frac{1}{T} \tag{8}$$

$$\left.\frac{\partial s}{\partial P}\right|_h \equiv s_P = \frac{-v}{T} \tag{9}$$

Note that the subscripts *P* and *h* refer to the partial derivatives with respect to these quantities when used as subscripts of entropy *s*. Using Equation 8, *T* can be defined as

$$T = \frac{1}{s_h} \tag{10}$$

Using the definition of ρ, and combining Equations 8 and 9,

$$\rho \equiv \frac{1}{v} = -\frac{s_h}{s_P} \tag{11}$$

Differentiating this expression with respect to *h* and *P* results in the following expressions:

$$\left.\frac{\partial \rho}{\partial h}\right|_P = \frac{\left(s_{hP}s_h - s_{hh}s_P\right)}{s_P^2} \tag{12}$$

$$\left.\frac{\partial \rho}{\partial P}\right|_h = \frac{\left(s_{PP}s_h - s_{hP}s_P\right)}{s_P^2} \tag{13}$$

Given the definition of *Cp*, and using the relationship for *T* in Equation 10,

$$Cp \equiv \left.\frac{\partial h}{\partial T}\right|_P = \frac{1}{\left.\frac{\partial T}{\partial h}\right|_P} = \frac{-1}{T^2\left.\frac{\partial(1/T)}{\partial h}\right|_P} = -\frac{s_h^2}{s_{hh}} \tag{14}$$

Similarly, given the relationship between *Cp* and *Cv*

$$Cp - Cv = -T\left.\left(\frac{\partial v}{\partial T}\right)^2\right|_P \left.\frac{\partial P}{\partial v}\right|_T \tag{15}$$

it can be shown that

$$Cv = \frac{-s_{hh}s_P^2 + 2s_{hP}s_h s_P - s_{PP}s_h^2}{s_{hh}s_{PP} - s_{hP}^2} \tag{16}$$

Finally, the value of the sonic velocity a can be derived from the fundamental definition

$$a = \frac{1}{\sqrt{\partial\rho/\partial P|_h + \left(\partial\rho/\partial h|_P/\rho\right)}} \tag{17}$$

using Equations 12 and 13.

The specific entropy (s) was then represented by piecewise-Hermite-interpolation double polynomials from which the properties and their derivatives were calculated. This single-function approach to the calculation of the thermodynamic properties and their derivatives ensures mathematical and thermodynamic consistency in the single-phase liquid and vapour regions.

The saturation properties are determined as a function of the absolute pressure (P). The saturation properties interpolated by piecewise cubic Hermite polynomials are:

$$h_v = f(P) \tag{18}$$

$$h_f = f(P) \tag{19}$$

$$T_{sat} = f(P) \tag{20}$$

$$\rho_v = f(P) \tag{21}$$

$$\rho_f = f(P) \tag{22}$$

where the subscripts v, f, and sat refer to the vapour, liquid, and saturated state of the substance respectively. The required saturation derivatives of these properties are determined through differentiation of the interpolation functions for consistency.

6. H_2O Thermodynamic Properties

In a non-equilibrium model of two-phase flow such as that used in CATHENA, thermodynamic property relations are required in both thermodynamic equilibrium states (subcooled liquid and superheated steam) and metastable states (superheated liquid and subcooled vapour). As a result, there are five distinct regions at sub-critical pressures, as shown in Figure 1:

1) Subcooled liquid (stable region)
2) Superheated liquid (metastable region)
3) Unstable region
4) Subcooled vapour (metastable region)
5) Superheated vapour (stable region)

The superheated liquid and subcooled vapour metastable state properties required were determined by extending the IAPWS analytical functions beyond the saturation state. Overall, the fitted properties provided by HLWP extend over a pressure range of 611.657 Pa to 100 MPa, and an enthalpy range of 0 to 17 MJ·kg^{-1} (or a temperature range of approximately 0 to 5000 °C), excluding the unstable region, as shown in Figure 1. For a given (P,h) input pair, the routines will provide values of T, ρ, $\partial\rho/\partial P|_h$, $\partial\rho/\partial h|_P$, Cp, Cv, a, and s. Although the temperature range extends to 5000 K, the properties do not account for the effects of dissociation on the properties at these temperatures.

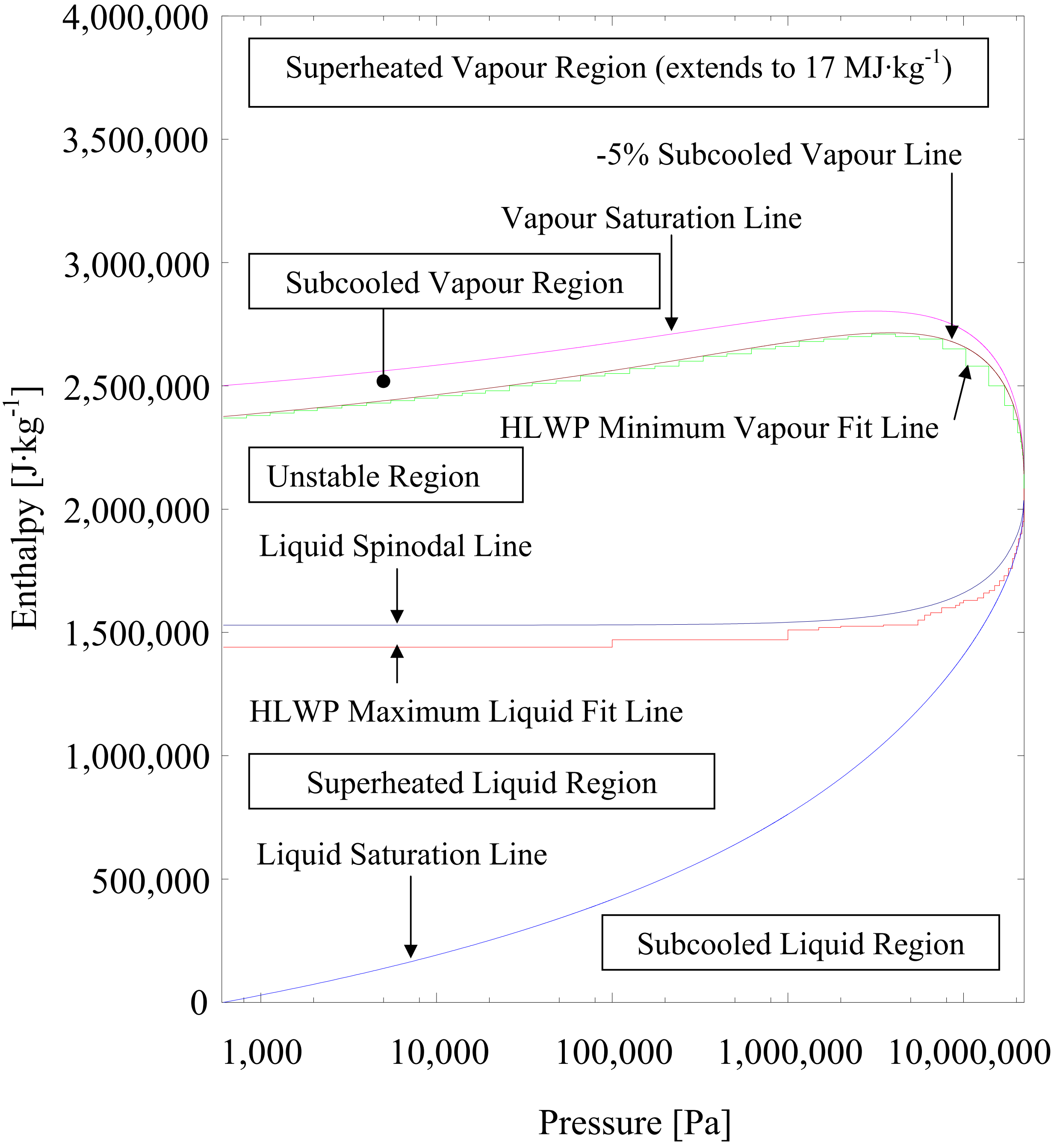

Figure 1 Fitted Regions for Subcritical Pressures.

A separate fit of the properties along the liquid and vapour saturation lines was also completed for the HLWP routines. Along the saturation lines, a cubic Hermite polynomial was used to fit the saturation values of T, and $\partial T/\partial P$, and the liquid and vapour saturation values of h, ρ, Cp, $\partial h/\partial P$, $\partial\rho/\partial P$ for a given value of pressure input. The saturation properties were fitted from a pressure of 611.657 Pa to 22.06399 MPa in both the liquid and the vapour phase.

As stated earlier, the HLWP routines smoothly extend into the supercritical region to a maximum pressure of 100 MPa. High accuracy fits of the supercritical properties are not difficult to achieve, as the properties and the change in their derivatives are relatively small. However, at pressures close to the critical point, some of the higher-order derivatives of entropy vary considerably with P or h, particularly those associated with the calculation of Cp. This makes it very difficult to achieve a fit that still produces acceptable accuracy in the immediate vicinity of the critical point. For this reason, the lower limit of the supercritical region was set to 22.0703 MPa, whereas the officially accepted critical point is 22.064 MPa. This is within 2σ of the error quoted for the critical point by the IAPWS formulation [3]. Thus the "critical point" in the HLWP routines occurs at a pressure of 22.0703 MPa and an enthalpy of 2084260 $\mathrm{J \cdot kg^{-1}}$. Since the pressure range from 22.064 to 22.0703 MPa is artificially placed in the subcritical region, requested saturation values in this region will be set to the saturation values at the last highest available fitted saturation point, 22.06399 MPa.

7. Testing of H_2O Thermodynamic Properties

Testing of the HLWP routines shows that the differences in the values of T, ρ, $\partial\rho/\partial P|_h$, $\partial\rho/\partial h|_P$, Cp, Cv, a, and s generated by HLWP and those produced by the IAPWS routines are less than 0.1% over the entire subcritical liquid and vapour regions as well as the supercritical region. The only exception to this are the HLWP fitted values of Cp, which can show differences of up to 0.23% with the IAPWS routines at the immediate vicinity of the critical point.

Testing of the saturation HLWP routines shows that the differences in the fitted HLWP values and those produced by the standard routines are less than 0.01% from a pressure of 611.657 Pa to 22.063 MPa. Over the 22.063 MPa to 22.06399 MPa pressure range the error is less than 1%. Stability and accuracy considerations of the IAPWS routines precluded fitting the saturation values exactly to the accepted critical pressure of 22.064 MPa.

Further internal consistency tests were also performed in which the saturation values were compared to the equivalent values generated by the biquintic fit values. The procedure involved choosing a pressure, and then extracting the saturation values from the saturation routines. The liquid and vapour saturation values of enthalpy along with the pressure were then used to obtain values of T, ρ_f, ρ_g, Cp_f, and Cp_g using the biquintic fit routines, and compared to the saturation values. In the pressure range below 17.9 MPa the saturation results compare to within 0.01% of the biquintic fit data. Above this pressure the agreement is not as good due to the fact that the biquintic fit grid does not always completely cover the saturation line as shown in Figure 1.

A final self-consistency check of the saturation fits for light water was also performed using the Clausius-Clapeyron relationship:

$$dP^{sat}/dT = (h_g - h_f) \,/\, [T\,(\,(1/\rho_g) - (1/\rho_f)\,)] \tag{23}$$

The variables needed to calculate both the left and right hand side of Equation 23 are generated by the HLWP saturation routines. If the saturation values are thermodynamically self-consistent, the left and right hand sides should agree with each other closely. In fact, when a detailed check is performed across the entire fitted saturation range, the maximum percentage difference is less than 0.0083%.

Finally, timing comparisons show that on the average over the entire spectrum of pressures and enthalpies, the HLWP routines are at least 1000 times faster than the IAPWS routines. The HLWP routines may be significantly faster than this in the regions close to the critical point.

8. H_2O Transport Properties

The analytical formulations for the transport properties of light water are implemented in HLWP-1.0 as follows:

1) The calculation of viscosity is based on the formulation described in an August 2003 IAPWS release [6],
2) The calculation of thermal conductivity is based on the formulation described in a September 1998 IAPWS release [7], and
3) The calculation of surface tension is based on the formulation reported in a September 1994 IAPWS release [8].

These standards have been directly implemented within HLWP to calculate the values of viscosity (μ), thermal conductivity (k), and surface tension (σ_s) for a given input (P,h).

The NIST routines for the calculation of μ, and k were directly implemented into HLWP-1.0 under subcritical and supercritical pressure conditions. The NIST routine for the calculation of σ_s was implemented directly into HLWP-1.0 under saturation conditions, and the saturation values of μ, and k were fit using piecewise cubic Hermite polynomial fits to the IAPWS routines.

The surface tension routine requires T_{sat} as an input. The value of T_{sat} is available from the HLWP routines for a given input pressure. Testing of the surface tension implementation was performed for input saturation pressure (P_{sat}) values by comparing the values of σ_s calculated using input values of T_{sat} derived using HLWP as well as the Bochum implementation of the IAPWS thermodynamic formulation. The difference between the HLWP-1.0 and the Bochum results was less than 2.38×10^{-6} N·m^{-1} over the entire pressure range.

The viscosity routine requires T, ρ, and $\partial\rho/\partial P|_T$ as inputs. The values of T and ρ are available from the present HLWP routines for a given input (P,h) pair. The calculation of $\partial\rho/\partial P|_T$ is also required. Since the HLWP routines provide the values $\partial\rho/\partial P|_h$, $\partial\rho/\partial h|_P$, s_{hh}, and s_{hP} it is possible to calculate $\partial\rho/\partial P|_T$ using the following relation:

$$\partial\rho/\partial P|_T=\partial\rho/\partial P|_h-(\partial\rho/\partial h|_P*(s_{hP}/s_{hh})) \tag{24}$$

The new formulation of the viscosity extends smoothly over a pressure range from the triple point at 611.657 Pa to 100 MPa and enthalpies from 0 MJ·kg^{-1} to 17 MJ·kg^{-1}. Testing of the viscosity implementation was performed for input (P,h) pair values by comparing the values of μ calculated using input values of T, ρ, and $\partial\rho/\partial P|_T$ derived using HLWP as well as the Bochum implementation of the IAPWS thermodynamic formulation. The maximum difference was 2.391×10^{-6} kg·s^{-1}·m^{-1} and the maximum percentage difference was 0.053% over the entire pressure and enthalpy range.

Verification of saturation fits for viscosity was performed for input P values by comparing values of μ calculated using the Bochum implementation of the IAPWS thermodynamic formulation with those calculated using the piecewise cubic Hermite polynomial fits in HLWP-1.0. The maximum difference was 9.08×10^{-9} kg·s^{-1}·m^{-1} and the maximum percentage difference was 0.0082% over the entire pressure range.

The thermal conductivity routine requires T, ρ, and $\partial P/\partial T|_\rho$ as inputs. The values of T and ρ are available from the HLWP routines for a given input (P,h) pair. The calculation of $\partial P/\partial T|\rho$ is also required. Since the HLWP routines provide the values $\partial\rho/\partial h|_P$, and Cp, and the value of $\partial\rho/\partial P|_T$

has already been calculated using Equation 24, it is possible to calculate $\partial P/\partial T|\rho$ using the following relation:

$$\partial P/\partial T|\rho = -((\partial \rho/\partial h|_P * Cp)/(\partial \rho/\partial P|_T)) \tag{25}$$

The new formulation of the thermal conductivity extends smoothly over a pressure range from the triple point at 611.657 Pa to 100 MPa and enthalpies from 0 MJ·kg^{-1} to 17 MJ·kg^{-1}. Testing of the thermal conductivity implementation was performed for input (P,h) values by comparing the values of k calculated using input values of T, ρ, and $\partial P/\partial T|\rho$ derived using HLWP as well as the Bochum implementation of the IAPWS thermodynamic formulation. The maximum difference was 3.901x10^{-3} W·m^{-1}·K^{-1} and the maximum percentage difference was 0.1% over the entire pressure and enthalpy range.

Testing of saturation fits for thermal conductivity was performed for input P values by comparing values of k calculated using the Bochum implementation of the IAPWS thermodynamic formulation with those calculated using the piecewise cubic Hermite polynomial fits in HLWP-1.0. The maximum difference was 5.9x10^{-5} W·m^{-1}·K^{-1} and the maximum percentage difference was 0.0012% over a pressure range from 611.657 Pa to 22.063 MPa. In the pressure range very close to the critical pressure (22.063 to 22.06399 MPa), the error in thermal conductivity is slightly higher as the value of the thermal conductivity becomes very large. In this pressure region, the maximum difference was 1.09x10^{-1} W·m^{-1}·K^{-1} and the maximum percentage difference was 0.23%.

9. Thermalhydraulic Calculations using Supercritical HLWP Property Routines

Prior to their inclusion into a prototype version of CATHENA, a test was performed on the light water property routines using driver subroutines. These routines calculated heat transfer coefficients applicable at super-critical pressures utilizing correlations selected from the open literature. The light water properties needed in the heat transfer correlations were obtained by exercising the HLWP-1.0 light water property routines. As shown in Figure 2, the calculated results are in good agreement with the experimental results. There were no difficulties experienced calculating heat transfer coefficients in the region in which the pressure (24.5 MPa) exceeds the critical pressure and crosses the line of pseudo-critical temperature (at a pressure of 24.5 MPa, the transition between quasi-liquid to quasi-vapour region occurs at about 656 K).

The HLWP-1.0 routines were also implemented into a prototype version of CATHENA for further testing. A water hammer simulation was performed using this version of CATHENA. The test consisted of a simple horizontal void collapse water hammer test in which the driving pressure was set to produce a large water hammer pressure excursion. As shown in Figure 3, there was no difficulty calculating water hammer pressure excursion in which the calculated pressures started in the subcritical region, and reached pressures of 24 MPa using the HLWP-1.0 property routines.

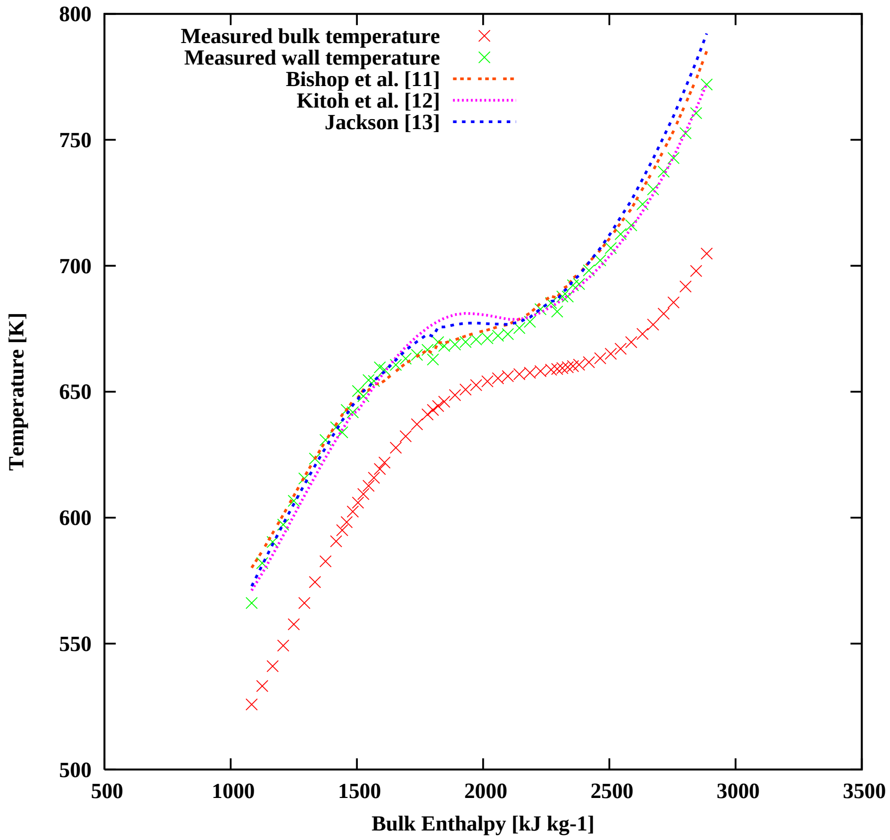

Figure 2 Comparison of experimental data [9,10], with predicted wall temperatures utilizing correlations [11,12,13] (tube, d=10 mm, water, P=24.5 Mpa, G=1180 kg m^{-2} s^{-1}, q=699 kW m^{-2})

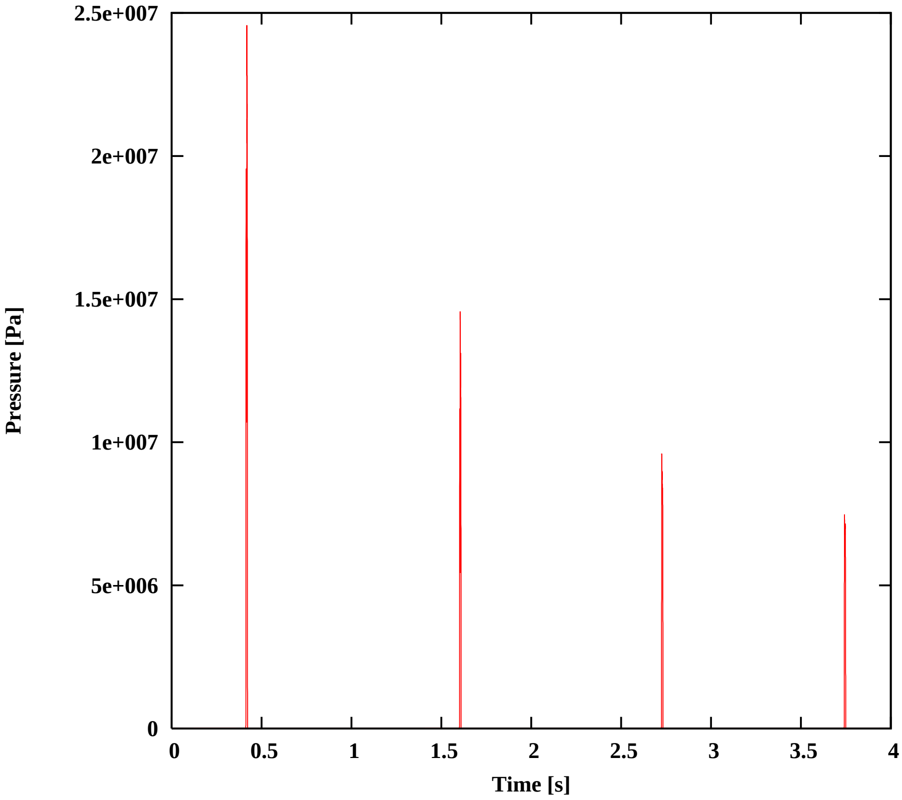

Figure 3 Water Hammer at Supercritical Pressures

10. Conclusions

Supercritical light water thermodynamic and thermophysical properties have been included into the HLWP-1.0 property routine library. Tests show that the routines are accurate to within 0.1% at pressures from 611.657 Pa to 100 MPa and enthalpies from 0 to 17 MJ·kg^{-1}. The exception is the generated value of *Cp*, which is accurate to within 0.23% at the immediate vicinity of the critical point. The saturation property routines are also accurate to within 0.01% at pressures from 611.657 Pa to 22.063 MPa and within 1% at pressures from from 22.063 to 22.06399 MPa. The thermophysical property routines are less than 0.1% different from the official IAPWS light water formulation. Tests show that the HLWP routines are at least 1000 times faster than the official IAPWS light water property routines. Implementation and testing of the HLWP-1.0 version demonstrates the property routines can be successfully and reliably utilized to perform thermalhydraulic simulations at supercritical conditions.

11. References

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