Appendix 1

Excerpt from [BIR60, pp73-74]:

Before taking up the main business of the chapter, we pause briefly to make a few comments regarding three kinds of time derivatives used in the text. We might illustrate them with a homely example—namely the problem of reporting the concentration of fish in the Kickapoo River. Because the fish are moving, the fish concentration c will be a function of position (x, y, z) and time (t).

The Partial Time Derivative, $\partial c/\partial t$

Suppose we stand on a bridge and note how the concentration of fish just below us changes with time. We are observing then how the concentration changes with time at a *fixed* position in space. Hence by $\partial c/\partial t$ we mean the "partial of c with respect to t, holding x, y, z constant."

Total Time Derivative, dc/dt

Suppose now that instead of standing on the bridge we get in a motorboat and speed around on the river, sometimes going upstream, sometimes across the current, and perhaps sometimes downstream. If we report the change of fish concentration with respect to time, the numbers we report must also reflect the motion of the boat. The total time derivative is given by

$$\frac{dc}{dt} = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x}\frac{dx}{dt} + \frac{\partial c}{\partial y}\frac{dy}{dt} + \frac{\partial c}{\partial z}\frac{dz}{dt}$$
(3.0-1)

in which dx/dt, dy/dt, and dz/dt are the components of the velocity of the boat.

Substantial Time Derivative. Dc/Dt

Suppose that we get into a canoe, and, not feeling energetic, we simply float along counting fish. Now the velocity of the observer is just the same as the velocity of the stream v. When we report the change of fish concentration with respect to time, the numbers depend on the local stream velocity. This derivative is a special kind of total time derivative and is called the "substantial derivative" or sometimes (more logically) the "derivative following the motion." It is related to the partial time derivative as follows:

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + v_x \frac{\partial c}{\partial x} + v_y \frac{\partial c}{\partial y} + v_z \frac{\partial c}{\partial z}$$
(3.0-2)

in which v_x , v_y , and v_x are the components of the local fluid velocity v.

The reader should thoroughly master the physical meaning of these three derivatives. Remember that $\partial c/\partial t$ is the derivative at a fixed point in space and Dc/Dt is a derivative computed by an observer floating downstream with the fluid.

APPENDIX 2

THE REYNOLDS TRANSPORT THEOREM (See "FUNDAMENTAL' MECHANICS OF FLUIDS, I.G. CURRIE, 1999-312.) 1974 199-3-12. Before deriving the theorem, let's get the nominclature straight: From the Eulerian point of views (fixed in space) a property, x, of a material (in this case, neutron density) is a function of time, t, and space, x, y, z But from a convective or Lagrangian point of view ~ is a function of t and the coordinates at to, ie Xo, yo, Zo. This means that given the starting point and the starting time, you can say where the -particle is at some later time, t. Now, Jollowing along the streamline or parte path with the same relacity as the particle, we notice a change, Sx. This change is due to a change in time only in Lagrangian system

and due to a change in space and time from the Eulerian point Spiew. So: $S \propto = \frac{\partial \alpha}{\partial t} St + \frac{\partial \alpha}{\partial x} Sx + \frac{\partial \alpha}{\partial y} Sy + \frac{\partial \alpha}{\partial z} Sz$ where the S refers to changes as seen in the Lagrangian system and the 2 refers to the more traditional change of a Junction of a number)) Junialdes as seen in traditional calculus and as we are used to in Eulerian formalisms. Durding by St : $\frac{\delta \alpha}{\delta t} = \frac{\partial \alpha}{\partial t} + \frac{\partial \alpha}{\partial x} \frac{\delta x}{\delta t} + \frac{\partial \alpha}{\partial y} \frac{\delta y}{\delta t} + \frac{\partial \alpha}{\partial z} \frac{\delta z}{\delta t},$ Qo $St \rightarrow 0$, $\frac{Sx}{St} \rightarrow \frac{D}{Pt}$, $\frac{Sx}{St} \rightarrow Velocity in x direction$ $<math>\frac{S}{St} \rightarrow \frac{D}{Pt}$, $\frac{Sx}{St} \rightarrow Velocity in x direction$ $<math>= V_x$ $\frac{2huo}{Dt} = \frac{\partial \alpha}{\partial t} + \frac{\sqrt{2}}{2} \nabla \alpha$ ground, you're seen this result before. This is just a reminder to reinforce the roots of the expression.

$$\frac{D}{Dt} \int \alpha(t) dt = \lim_{\delta t \to 0} \left\{ \frac{1}{\delta t} \left[\int_{\Psi(t+\delta t)} \alpha(t+\delta t) dt - \int_{\Psi(t)} \alpha(t+\delta t) dt - \int_{\Psi(t)} \alpha(t+\delta t) dt \right] \right\}$$

$$= \lim_{\substack{\delta t \to 0}} \left\{ \int_{\delta t} \left[\int_{V(t)}^{\infty} \alpha(t+\delta t) dt - \int_{V(t)}^{\infty} \alpha(t+\delta t) dt - \int_{V(t)}^{\infty} \alpha(t) dt - \int_{V$$

•

To
$$\frac{b}{Dt} \int_{V(t)} (x(t)) dt = \lim_{St \to 0} \left\{ \frac{d}{St} \left[\int_{V(t+St) - V(t)} dt \right] \right\} + \int_{V(t)} \frac{dx}{dt} dt$$

The remaining limit corresponds to the volume
changing while a remains constant.
Consider the volume as it moves and changes
shape:
 $V(t)$
 t
 $V(t)$
 $V(t)$
 t
 $V(t)$
 t
 $V(t)$
 t
 $V(t)$
 t
 $V(t)$
 t
 $St = \underbrace{V \cdot \underline{n} St}_{St}$
 Dt
 $\int_{V(t)} (x(t)) dt = \underbrace{J \cdot \underline{n} (t) dt}_{V(t)} dt$
 Dt
 $\int_{V(t)} (x(t)) dt = \underbrace{J \cdot \underline{n} (t) dt}_{St} + \underbrace{J \cdot \underline{n} ds}_{St}$.

•

Of course, we can replace the surface integral with a volume integral using Souss' Theorem to get: $\frac{D}{Dt}\int_{\Psi} \propto d\Psi = \int_{\Psi} \left[\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \underline{V}) \right] d\Psi \cdot$ These last two expressions of Reynold's Transport Theorem give up a neat way to take derivatives involving varying integrands. Alike this derivation by Currie because it helps to generate some institution on the physical processes involved.

asyon might have expected. This is not the only way to generate this result. For instance, we could listen to Truecdell:

APPENDIX 3 Rearrangement of independent voriatles. Ĵ X = X(P,T)Y = Y(P,T)P = P(P,T)h = h(P,T)quien we often need. $\left(\frac{\partial Y}{\partial x}\right)_{P}$ or $\left(\frac{\partial Y}{\partial x}\right)_{T}$ or $\left(\frac{\partial Y}{\partial P}\right)_{X}$ etc We can easily rearrange as follows: step 1: expand ! $dx = \frac{dx}{dp} + qb + \frac{dx}{dT} + \frac{dx}{dT}$ $dY = \frac{\partial X}{\partial P} + \frac{\partial P}{\partial T} + \frac{\partial Y}{\partial T} = \frac{\partial T}{\partial T}$ styp2: solve for dP ddT ... $dP = \frac{\partial Y}{\partial T} dx - \frac{\partial X}{\partial T} dy$ $\frac{\partial x}{\partial \varphi} \left(\frac{x \varepsilon}{\tau \delta} - \frac{\partial y}{\partial \tau \delta} \right)_{\tau} \left(\frac{x \varepsilon}{\tau \delta} \right)_{\tau}$ <u>dy</u> dx - dx dy dT = $-\left[\frac{\partial x}{\partial r}\right]_{\tau} - \frac{\partial y}{\partial \tau} - \frac{\partial y}{\partial \tau} - \frac{\partial y}{\partial \tau} = -\frac{\partial y}{\partial \tau} + \frac{\partial y}{\partial \tau} = -\frac{\partial y}{$

Selected differentials from a condensed collection of thermodynamic formulas by P. W. Bridgman

Any partial derivative of a state variable of a thermodynamic system, with respect to any other state variable, a third variable being held constant [for example, $(\partial u/\partial v)_T$] can be written, from Eq. (4-20), in the form

$$(\partial u/\partial v)_T = \frac{(\partial u/\partial z)_T}{(\partial v/\partial z)_T}$$

where z is any arbitrary state function. Then if one tabulates the partial derivatives of all state variables with respect to an arbitrary function z, any partial derivative can be obtained by dividing one tabulated quantity by another. For brevity, derivatives of the form $(\partial u/\partial z)_T$ are written in the table below in the symbolic form $(\partial u)_T$. Then, for example,

$$\left(\frac{\partial u}{\partial v}\right)_T = \frac{(\partial u)_T}{(\partial v)_T} = \frac{T(\partial v/\partial T)_{I'} + P(\partial v/\partial P)_T}{-(\partial v/\partial P)_T} = \frac{T\beta}{\kappa} - P,$$

which agrees with Eq. (6-9). Ratios (not derivatives) such as $d'q_P/dv_P$ can be treated in the same way. For a further discussion, see A Condensed Collection of Thermodynamics Formulas by P. W. Bridgman (Harvard University Press, 1925), from which the table below is taken.

P constant T constant $(\partial P)_T = -1$ $(\partial T)_{\rm P} = 1$ $(\partial v)_{i} = (\partial v / \partial T)_{i}$ $(\partial v)_{T} = -(\partial v/\partial P)_{T}$ $(\partial s)_{II} = c_{II}/T$ $(\partial s)_T = (\partial v / \partial T)_I$ $(\partial q)_T = T(\partial v/\partial T)_P$ $(\partial q)_{II} = c_{II}$ $(\partial w)_P = P(\partial v/\partial T)_P$ $(\partial w)_T = -p(\partial v/\partial P)_T$ $(\partial u)_{\tau} = T(\partial v/\partial T)_{\nu} + P(\partial v/\partial P)_{\tau}$ $(\partial u)_P = c_P - P(\partial v/\partial T)_P$ $(\partial h)_{P} \neq c_{P}$ $(\partial h)_T = -v + T(\partial v/\partial T)_P$ $(\partial g)_{P} = -s$ $(\partial g)_T = -v$ $(\partial f)_P = -s - P(\partial v / \partial T)_{i}$ $(\partial f)_T = P(\partial v/\partial P)_T$

h constant

(

$$\partial P)_{h} = -c_{P}$$

$$\partial T)_{h} = v - T(\partial v/\partial T)_{P},$$

$$\partial v)_{h} = -c_{P}(\partial v/\partial P)_{T} - T(\partial v/\partial T)_{P}^{2},$$

$$+ v(\partial v/\partial T)_{P},$$

 $(\partial s)_h = vc_P/T$

 $(\partial q)_h = vc_P$ $(\partial w)_h = -P[c_P(\partial v/\partial P)_T + T(\partial v/\partial T)_P^*]$ $-v(\partial v/\partial T)_P]$

 $\frac{s \text{ constant}}{(\partial P)_{i}} = -c_{P}/T$ $(\partial T)_{i} = -(\partial v/\partial T)_{P}$ $(\partial v)_{s} = -\frac{1}{T} [c_{P}(\partial v/\partial P)_{T} + T(\partial v/\partial T)_{I}^{2}]$ $(\partial q)_{s} = 0$ $(\partial w)_{s} = -\frac{P}{T} [c_{P}(\partial v/\partial P)_{T} + T(\partial v/\partial T)_{I}^{2}]$ $(\partial u)_{s} = \frac{P}{T} [c_{P}(\partial v/\partial P)_{T} + (T \partial v/\partial T)_{I}^{2}]$ $(\partial k)_{s} = -vc_{P}/T$ $(\partial g)_{s} = -\frac{1}{T} [vc_{P} - sT(\partial v/\partial T)_{I}]$ $(\partial f)_{s} = \frac{1}{T} [Pc_{P}(\partial v/\partial P)_{T} + PT(\partial v/\partial T)_{I}^{2}]$ $+ sT(\partial v/\partial T)_{I}]$

g constant $(\partial P)_{g} = s$ $(\partial T)_{g} = v$ $(\partial v)_{g} = v (\partial v/\partial T)_{P} + s(\partial v/\partial P)_{T}$

$$(\partial s)_{\sigma} = \frac{1}{T} [vc_{P} - sT(\partial v/\partial T)_{P}]$$

$$(\partial q)_{\sigma} = -sT(\partial v/\partial T)_{P} + vc_{P}$$

$$(\partial w)_{\sigma} = P[v(\partial v/\partial T)_{P} + s(\partial v/\partial P)_{T}]$$

 $\frac{v \text{ constant}}{(\partial P)_v} = -(\partial v/\partial T)_I.$ $(\partial T)_n = (\partial v/\partial P)_T$ $(\partial s)_v = \frac{1}{T} [c_I(\partial v/\partial P)_T + T(\partial v/\partial T)_I^{\dagger}.]$ $(\partial q)_v = c_I.(\partial v/\partial P)_T + T(\partial v/\partial T)_I^{\dagger}.$ $(\partial w)_v = 0$ $(\partial u)_v = c_I.(\partial v/\partial P)_T + T(\partial v/\partial T)_I^{\dagger}.$ $(\partial h)_v = c_I.(\partial v/\partial P)_T + T(\partial v/\partial T)_I^{\dagger}.$ $(\partial h)_v = c_I.(\partial v/\partial P)_T + T(\partial v/\partial T)_I^{\dagger}.$ $(\partial g)_v = -v(\partial v/\partial T)_I. - s(\partial v/\partial P)_T$ $(\partial f)_v = -s(\partial v/\partial P)_T$

APPENDIX 4

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APPROXIMATE FUNCTIONS FOR THE FAST CALCULATION OF LIGHT-WATER PROPERTIES AT SATURATION

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Abstract--For thermalhydraulic systems analysis, linear interpolation algorithms are commonly used for the calculation of thermodynamic properties. However, these algorithms can use a substantial amount of computer time and memory. An alternative to this approach suggested in the past is the use of approximation formulas. Such formulas for the calculation of the thermodynamic properties of light water for saturation conditions are presented here, based on the 1984 NBS/NRC Steam Tables. The range of these approximations is from below 1b to just below the critical point (22.055 MPa) with a deviation from tabulated values of not more than 0.22%. The formulas were determined by the ratehod of least squares, enabling a minimization of deviations from the line of best fit and the fitting of functions simple enough to be used with programmable calculators, as well as microcomputers. In addition to the rapid calculation of the properties, the simple curve fits are instrumental in the development of the rate form of the equation of state.

Since any given property cannot be accurately fitted over the entite pressure range with a single simple expression, the pressure range was split into subranges. Special care was taken to ensure that the slopes of the curve fits were continuous across the boundaries since discontinuities in the slopes of the property tables can cause instabilities and failure of search algorithms in typical computer codes.

Key Words: water properties, curve fit, fast, saturation.

INTRODUCTION

In the analysis of flow systems, the thermodynamic properties are usually calculated by linear interpolation algorithms applied to thermodynamic tables stored on computer. However, the storage of these steam tables can occupy a large amount of computer memory. As well, the linear interpolation algorithms require a searching algorithm to select the proper numbers from the tables. Thus the use of such algorithms can considerably tax computer running time. An alternative to this method is the employment of approximate formulas, similar to those described by Firla (1984), which can rapidly compute the value of a property with satisfactory accuracy for the purpose of system analysis.

This paper concentrates on the thermodynamic properties of light water for saturation conditions. At saturation, the temperature can be expressed as a function of pressure only. Therefore, we can represent the properties by a number of simple functions containing one independent variable; pressure.

In addition to the direct calculation of thermodynamic properties, these approximation functions can be applied to the determination of the rate form of the equation of state (Garland & Sollychin 1988).

APPROXIMATION METHOD

The approach taken in developing the correlations minimized the deviations from the reference steam tables. To maintain a high accuracy it was necessary to subdivide the range of pressure variation into several regions. The simple functions used were fitted to the data by the method of least squares, as discussed in the following section.

As system codes often require the slopes of the properties, the fits to the steam table by a set of approximation functions, were required to exhibit a continuous first derivative across the entire range of pressure.

Least-squares method

We represent a set of *n* data points by some relationship y = f(x), containing *p* unknown parameters a_1, a_2, \ldots, a_p , the deviations or residuals are given by

$$D_i = f(\mathbf{x}_i) - \mathbf{y}_i. \tag{1}$$

The sum of the squares of the deviations,

$$S = \sum_{i=1}^{n} D_i^2 \stackrel{c}{=} \sum_{i=1}^{n} [f(x_i) - y_i]^2, \qquad [2]$$

is a function of a_1, a_2, \ldots, a_p . The parameters are determined such that S is a minimum $(dS/dc_1 = 0, dS/da_2 = 0, \ldots, dS/da_p = 0)$.

If we take y = f(x) to be a linear function $(y = a_1 + a_2 x)$, the residuals are $D_i = (a_1 + a_2 x_i) - y_i$, so that

$$S = (a_1 + a_2 x_1 - y_1)^2 + (a_1 + a_2 x_2 - y_2)^2 + \ldots + (a_1 + a_2 x_n - y_n)^2.$$
 [3]

On differentiating S with respect to a_1 and a_2 , two equations are obtained:

$$\frac{dS}{da_1} = 2(a_1 + a_2x_1 - y_1) + 2(a_1 + a_2x_2 - y_2) + \ldots + 2(a_1 + a_2x_n - y_n) = 0$$

and

$$\frac{\mathrm{d}S}{\mathrm{d}a_2} = 2(x_1)(a_1 + a_2x_1 - y_1) + 2(x_2)(a_1 + a_2x_2 - y_2) + \ldots + 2(x_n)(a_1 + a_2x_n - y_n) = 0$$
 [4]

Dividing by two and collecting the coefficients of a_1 and a_2 , we get

$$na_1 + \left(\sum_{i=1}^n x_i\right)a_2 = \sum_{i=1}^n y_i$$

and

$$\left(\sum_{i=1}^{n} x_{i}\right)a_{i} + \left(\sum_{i=1}^{n} x_{i}^{2}\right)a_{2} = \sum_{i=1}^{n} x_{i}y_{i}.$$
[5]

Similarly, for a second-order polynomial (quadratic equation):

$$4a_1 + \left(\sum_{i=1}^n x_i\right)a_2 + \left(\sum_{i=1}^n x_i^2\right)a_3 = \sum_{i=1}^n y_i,$$
 [6a]

$$\left(\sum_{i=1}^{n} x_{i}\right)a_{1} + \left(\sum_{i=1}^{n} x_{i}^{2}\right)a_{2} + \left(\sum_{i=1}^{n} x_{i}^{3}\right)a_{3} = \sum_{i=1}^{n} x_{i}y_{i},$$
[6b]

and

$$\left(\sum_{i=1}^{n} x_{i}^{2}\right)a_{i} + \left(\sum_{i=1}^{n} x_{i}^{3}\right)a_{2} + \left(\sum_{i=1}^{n} x_{i}^{4}\right)a_{3} = \sum_{i=1}^{n} x_{i}^{2}y_{i}.$$
 [6c]

These equations can be solved for a_1 , a_2 and a_3 to give the function $y = a_1 + a_2 x + a_3 x^2$. Higher order polynomials may also be fitted in this manner, of course.

Correlations are often described by a correlation constant, r. This number expresses the strength and direction of the correlation and can vary from +1.00 to -1.00. For positive correlations where an increase in one variable tends to lead to an increase in the other variable being considered, r is positive. For negative correlations where an increase in one variable tends to lead to a decrease in the other, r is negative. The largest magnitude of r is 1.00 which represents a perfect correlation. Thus the closer the points in a plot of the two variables come to falling on the line of best fit, the nearer r will be to +1.00 or -1.00. The following section describes different types of functions that can be determined using the method of least squares. The correlation constant can be used as a way to compare each function and to see if the range being fitted is too large to obtain a high enough accuracy with the steam tables.

Table 1. Transforming functions into a linear form

Function	Operations on data	Linear form
$\frac{a}{a+b}$	1 x == -	$y = q\left(\frac{1}{2}\right) + b$
y = x + 0) = = (x) + v
$y = ax^b$	$y \Rightarrow \log y$	$(\log y) = b(\log x) + \log a$
$y = a \exp(bx)$	$y \Rightarrow \log y$	$(\log y) = bx + \log a$
$y = a \log x + b$	x⇒log x	$y = a(\log x) + b$

The correlation constant for y = ax + b is calculated as

$$r = \frac{b \sum_{i=1}^{n} y_i + a \sum_{i=1}^{n} (x_i y_i) - \frac{\left(\sum_{i=1}^{n} y_i\right)^2}{n}}{\sum_{i=1}^{n} (y_i)^2 - \frac{\left(\sum_{i=1}^{n} y_i\right)^2}{n}}$$
[7]

Similarly, for $y = ax^2 + bx + c$,

$$r = \frac{c\sum_{i=1}^{n} y_i + b\sum_{i=1}^{n} (x_i y_i) + a\sum_{i=1}^{n} (x_i^2 y_i) - \frac{\left(\sum_{i=1}^{n} y_i\right)^2}{n}}{\sum_{i=1}^{n} (y_i)^2 - \frac{\left(\sum_{i=1}^{n} y_i\right)^2}{n}}$$
[8]

Using least squares for other functions

Data can be approximated by other functions which include power, exponential and logarithmic forms. The coefficients of each of these functions can be determined using [5] by altering the data, as shown in table 1, to transform the functions into a linear form. The power function and the exponential function are expected to be useful in producing an accurate curve fit of the thermodynamic properties. However, the method of least squares determines these functions such that x = 0 for y = 0. To obtain better accuracy with these curves, we can shift the data by adding to or subtracting from the x and y values. For example, figure 1(a) shows two curves passing



Figure 1. Example of data shifting. (a) The solid line represents the best-fit curve as determined by sight. The dashed line represents the best-fit power curve as determined by the method of least squares. (b) The y values in (a) have a constant value, Y_0 , subtracted from them such that the solid line passes through the origin. The dashed line is now more comparable to the solid line and is given by $y - Y_0 = ax^b$, where a and b are found using [5].



Figure 2. Dealing with negative sloping curves. (a) The actual data points are plotted. The slope of a curve passing through these points is negative. From figure 1, one can see that the shift that would produce the most accurate fit makes all $(y - Y_0)$ values negative in this case. (b) The negative y values are plotted here. The slope of a curve passing through these points is positive (c) The negative y values are shifted upward by a constant, Y_0 , such that all $y'' = -y + Y_0$ are positive. The method of least squares can now be used for the power and exponential functions. For the power function, the equation determined by least squares is given by $y = Y_0 - ax^b$.

through a set of points. Curve 1 is the best fit, as determined by sight, and curve 2 is the best fit of a power function, as determined by the method of least squares, without shifting the data. Figure 1(b) shows the two curves after a constant, Y_0 , has been subtracted from each y value. We can see the effectiveness of a shifting of data. By comparing the correlation constants for different shifts, one can determine which shift gives the most accurate curve fit. The shifting of the data should be done before the operations described in table 1 are carried out.

In some circumstances, such as when there is a decrease in y for an increase in x, the necessary shifting of data would produce negative values either in the x or y direction. To avoid taking the log of a negative number we can fit the negative of the y values. Figure 2 demonstrates this procedure.

CORRELATIONS OF LIGHT-WATER THERMODYNAMIC PROPERTIES[†]

The following thermodynamic properties of light water at saturation were fitted to approximation functions: (1) specific volume/density, (2) specific enthalpy, (3) saturation temperature, (4) specific entropy, (5) specific heat and (6) dynamic viscosity. The reference source of data for all of these properties, with the exception of viscosity, is the NBS/NRC Steam Tables (Haar et al. 1984). The subroutines by Sokolnikoff & Redheffer (1966) were used for the calculation of the above properties.

These subroutines were also used in conjunction with the equation for viscosity given by White (1975/1983). This combination was shown to yield an adequate representation of viscosity by Kamgar-Parsi & Sengers (1982).

The set of functions for each property are listed along with their range of use and the worst accuracy encountered over this range. Figures 3-13 show the properties and the accuracy of the approximation, as calculated by

$$\operatorname{accuracy} = \frac{Y_{\operatorname{approx}} - Y_{\operatorname{steam (ables)}}}{Y_{\operatorname{steam (ables)}}} * 100 [\%].$$
[9]

For all of the properties, the range of each function was chosen such that the accuracy is as small as possible and the first derivatives of two adjoining functions are equal at the point where they

[†]Program diskettes, containing the programs used in the determination of the approximation functions and in the reproduction of property tables, can be obtained from the first author. These diskettes are available in either PDP11 or IBM-PC format.

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Figure 3. Specific volume of the liquid phase at saturation.



Figure 5. Specific enthalpy of the liquid phase at saturation







Figure 6. Specific enthalpy of the vapor phase at saturation.



Figure 7. Saturation temperature.

join. Thus the sets of functions for specific volume and specific enthalpy can be used for the calculation of the rate form equation of state (Garland & Sollychin 1988) and in computer algorithms involving the Jacobi of the system matrix. The continuity of the slopes for specific volume (liquid phase), density (gas phase) and specific enthalpy for both phases, is shown in figures 14-17.

The approximation functions can now be applied to the rate form of the equation of state (see the appendix). Plots of the F functions of [A.2] are shown in figures 13-22. Each of the F functions yields a smooth continuous curve, as desired.

Specific volume, liquid phase at saturation

The functions given below are an approximation to the specific volume of light water in the liquid phase, v_L [m³/kg], for saturation conditions. The pressure range within which they may be used is 0.075–21.5 MPa with the accuracy not worse than 0.14%. Figure 3 shows the accuracy of the approximation.

Approximation functions:

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 $v_{L} = 1.2746977E - 4 * P ** (0.4644339) + 0.001$ $0.075 MPa \leq P \leq 1.00 MPa$ $v_{L} = 1.0476071E - 4 * P ** (0.5651090) + 0.001022$ $1.00 MPa < P \leq 3.88 MPa$ $v_{L} = 3.2836717E - 5 * P + 1.12174735E - 3$ $3.88 MPa < P \leq 8.84 MPa$ $v_{L} = 3.3551046E - 4 * \exp(5.8403566E - 2 * P) + 0.00085$ $8.84 MPa < P \leq 14.463 MPa$ $v_{L} = 3.1014626E - 8 * P ** (3.284754) + 0.00143$ 14.463 MPa < P < 18.052 MPa $v_{L} = 1.5490787E - 11 * P ** (5.7205) + 0.001605$ $18.052 MPa \leq P < 20.204 MPa$ $v_{L} = 4.1035988E - 24 * P ** (15.03329) + 0.00189$ $20.204 MPa \leq P \leq 21.5 MPa.$

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Figure 8. Specific entropy of the liquid phase at saturation.



Figure 10. Specific heat of the liquid phase at saturation.



Figure 9. Specific entropy of the vapor phase at saturation.



Figure 11. Specific heat of the vapor phase at saturation.



Figure 12. Viscosity of the liquid phase at saturation.



Figure 14. The slope of the specific volume of the liquid phase at saturation.

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10.0

PRESSURE (MPa)

14.0

22.0

18.0

6.0

20.0

10.0

0.0

2.0



Figure 16. The slope of the specific enthalpy of the liquid phase at saturation.



Figure 17. The slope of the specific enthalpy of the vapor phase at saturation.

Density, gas phase at saturation

The following correlations give an approximation to the density of light water in the gas phase, $D_{\rm G}[\rm kg/m^3]$, for saturation conditions. Their range of use is 0.085-21.5 MPa with the accuracy net worse than 0.22%. Figure 4 shows the accuracy of the approximation.

 $\begin{array}{l} Approximation \ functions:\\ \\ D_{G}=5.126076*P**(0.9475862)+0.012\\ 0.085\ MPa < P < 1.112\ MPa\\ \\ D_{G}=4.630832*P**(1.038819)+0.52\\ 1.112\ MPa \leqslant P < 3.932\ MPa\\ \\ D_{G}=2.868721*P**(1.252148)+3.80\\ 3.932\ MPa \leqslant P < 8.996\ MPa\\ \\ D_{G}=0.5497553*P**(1.831182)+18.111\\ 8.996\ MPa \leqslant P < 14.628\ MPa\\ \\ D_{G}=8.5791582E-3*P**(3.176484)+50.0\\ 14.628\ MPa \leqslant P \leqslant 18.21\ MPa\\ \\ D_{G}=3.5587113E-6*P**(5.660939)+88.0\\ 18.21\ MPa < P \leqslant 20.253\ MPa\\ \\ D_{G}=3.558734E-16*P**(13.03774)+138.0\\ 20.253\ MPa < P \leqslant 21.5\ MPa.\\ \end{array}$

Specific enthalpy, liquid phase at saturation

The correlations given below approximate the specific enthalpy of light water in the liquid phase. $h_L[kJ/kg]$, for saturation conditions. The range for which they may be used is 0.075-21.70 MPa with the accuracy not worse than 0.10%. Figure 5 shows the accuracy of the approximation.

Approximation functions:

 $h_{\rm L} = 912.1779 * P ** (0.2061637) - 150.0$

0.075 MPa < P < 0.942 MPa



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Figure 22. The function F_5 .

 $\begin{aligned} h_{\rm L} &= 638.0621 * P ** (0.2963192) + 125.0 \\ &0.942 \,{\rm MPa} \leqslant P < 4.02 \,{\rm MPa} \\ h_{\rm L} &= 373.7665 * P ** (0.4235532) + 415.0 \\ &4.02 \,{\rm MPa} \leqslant P < 9.964 \,{\rm MPa} \\ h_{\rm L} &= 75.38673 * P ** (0.8282384) + 900.0 \\ &9.964 \,{\rm MPa} \leqslant P < 16.673 \,{\rm MPa} \\ h_{\rm L} &= 0.1150827 * P ** (2.711412) + 1440.0 \\ &16.673 \,{\rm MPa} \leqslant P < 20.396 \,{\rm MPa} \\ h_{\rm L} &= 9.1417257E - 14 * P * (11.47287) + 1752.0 \\ &20.396 \,{\rm MPa} \leqslant P \leqslant 21.70 \,{\rm MPa}. \end{aligned}$

Specific enthalpy, gas phase at saturation

The following functions give an approximation of the specific enthalpy of light water in the gas phase, $h_G[kJ/kg]$, for saturation conditions. Their range is 0.075-21.55 MPa with the accuracy not worse than 0.066%. Figure 6 shows the accuracy of the approximation.

Approximation functions:

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$$\begin{split} h_{\rm G} &= -4.0381938\mathrm{E} - 6*(3.0-P)**(15.72364) + 2750.0\\ &0.075\ \mathrm{MPa}$$

$$h_{\rm G} = -3.532177*(P - 8.00)**2.0 + 29.81305*(P - 8.00) + 2565.00$$

$$16.497 \text{ MPa} \leq P < 20.193 \text{ MPa}$$

$$h_{\rm G} = -22.92521*(P - 18.0)**2.0 + 44.23671*(P - 18.0) + 2415.01$$

$$20.193 \text{ MPa} \leq P \leq 21.55 \text{ MPa}.$$

Saturation temperature

The correlations given below are for the saturation temperature of light water, T_{ut} [°C]. The pressure range for which they may be used is 0.070-21.85 MPa with the accuracy not worse than 0.02%. Figure 7 shows the accuracy of the approximation.

Approximation functions:

 $T_{\text{sat}} = 236.2315 * P ** (0.1784767) - 57.0$ $0.070 \text{ MPa} \leq P < 0.359 \text{ MPa}$ $T_{\text{sat}} = 207.9248 * P ** (0.2092705) - 28.0$ $0.359 \text{ MPa} \leq P \leq 1.676 \text{ MPa}$ $T_{\text{sat}} = 185.0779 * P ** (0.2323217) - 5.0$ $1.676 \text{ MPa} < P \leq 8.511 \text{ MPa}$ $T_{\text{sat}} = 195.1819 * P ** (0.2241729) - 16.0$ 8.511 MPa < P < 17.69 MPa $T_{\text{sat}} = 227.2963 * P ** (0.201581) - 50.0$

$$17.69 \text{ MPa} \leq P \leq 21.85 \text{ MPa}$$

Specific entropy, liquid phase at saturation

The functions given below are an approximation of the specific entropy of light water in the liquid phase. $s_L[kJ/kg]$, for saturation conditions. Their range of use is 0.065-21.25 MPa with the accuracy not worse than 0.12%. Figure 8 shows the accuracy of the approximation.

Approximation functions:

 $s_{L} = 3.340244 * P ** (0.125474) - 1.20$ $0.065 \text{ MPa} \leq P < 1.666 \text{ MPa}$ $s_{L} = 1.748203 * P ** (0.2275611) + 0.40$ $1.666 \text{ MPa} \leq P < 8.825 \text{ MPa}$ $s_{L} = 0.2549248 * P ** (0.6381866) + 2.25$ $8.325 \text{ MPa} \leq P < 16.66 \text{ MPa}$ $s_{L} = 4.3632383E - 5 * (P - 0.40) ** (3.153273) + 3.50$ $16.66 \text{ MPa} \leq P < 21.25 \text{ MPa}.$

Specific entropy, gas phase at saturation

The following functions give an approximation to the specific entropy of light water in the gas phase, $s_G[kJ/kg]$, for saturation conditions. Their range is 0.025-21.50 MPa with the accuracy not worse than 0.10%. Figure 9 shows the accuracy of the approximation.

Approximation functions:

 $s_{\rm G} = 6.58681 - 0.335924 * \log(P)$ 0.025 MPa $\leq P \leq 1.48$ MPa

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$$\begin{split} s_{\rm G} &= 7.80 - 1.227644 * P ** (0.2481072) \\ & 1.48 \ {\rm MPa} < P \leqslant 8.05 \ {\rm MPa} \\ s_{\rm G} &= 6.30 - 0.084638514 * P ** (0.9082161) \\ & 8.05 \ {\rm MPa} < P \leqslant 15.64 \ {\rm MPa} \\ s_{\rm G} &= 5.50 - 3.6897161E - 3*(P - 7.80) ** (2.012466) \\ & 15.64 \ {\rm MPa} < P \leqslant 20.00 \ {\rm MPa} \\ s_{\rm G} &= 5.00 - 0.042830642 * (P - 18.7) ** (1.779526) \\ & 20.00 \ {\rm MPa} < P \leqslant 21.5 \ {\rm MPa}. \end{split}$$

Specific heat, liquid phase at saturation

The correlations given below are an approximation to the specific heat of light water in the liquid phase, $C_{PL}[kJ/kg K]$, for saturation conditions. Their range of use is 0.030-20.3 MPa. For pressures <13.3 MPa, the accuracy is not worse than 0.08%; for pressures >13.3 MPa, the error can be as high as 0.60%. Figure 10 shows the accuracy of the approximation.

 $\begin{array}{l} \textit{Approximation functions:}\\ C_{pL} = 0.247763*P**(0.5704026) + 4.150\\ 0.030 \ \text{MPa} \leqslant P < 0.671 \ \text{MPa}\\ C_{pL} = 0.179305*P**(0.8967323) + 4.223\\ 0.671 \ \text{MFa} \leqslant P < 2.606 \ \text{MPa}\\ C_{pL} = 0.09359843*P**(1.239114) + 4.340\\ 2.606 \ \text{MPa} \leqslant P < 6.489 \ \text{MPa}\\ C_{pL} = 0.01068888*P**(2.11376) + 4.740\\ 6.489 \ \text{MPa} \leqslant P < 11.009 \ \text{MPa}\\ C_{pL} = 1.333058E - 4*P**(3.707294) + 5.480\\ 11.009 \ \text{MPa} \leqslant P < 14.946 \ \text{MPa}\\ C_{pL} = 6.635658E - 3*(P - 10.0)**(3.223323) + 7.350\\ 14.946 \ \text{MPa} \leqslant P < 18.079 \ \text{MPa}\\ C_{pL} = 4.6844786E - 6*\exp(0.7396875*P) + 10.020\\ 18.079 \ \text{MPa} \leqslant P \leqslant 20.30 \ \text{MPa}. \end{array}$

Specific heat, gas phase at saturation

The following correlations give an approximation to the specific heat of light water in the gas phase, $C_{pG}[kJ/kg K]$, for saturation conditions. Their range of use is 0.050-20.40 MPa. For pressures < 16.0 MPa, the accuracy is not worse than 0.12%; for pressures > 16.0 MPa, the error can be as high as 0.60%. Figure 11 shows the accuracy of the approximation.

Approximation functions:

$$\begin{split} C_{pG} &= 0.6471635 * (P - 0.006) * * (0.6400569) + 1.90 \\ &\quad 0.050 \text{ MPa} \leqslant P \leqslant 0.599 \text{ MPa} \\ C_{pG} &= 0.5560633 * P * * (0.8197355) + 2.00 \\ &\quad 0.599 \text{ MPa} \leqslant P < 2.391 \text{ MPa} \end{split}$$

$$\begin{split} C_{pG} &= 0.3187082*P**(1.110271)) \pm 2.30\\ &2.391 \text{ MPa} \leqslant P < 5.661 \text{ MIPa}\\ C_{pG} &= 0.064275995*P**(1.766106) \pm 3.12\\ &5.661 \text{ MPa} \leqslant P < 9.458 \text{ MIPa}\\ C_{pG} &= 3.8011048E - 3*P**(2.816397) \pm 4.40\\ &9.458 \text{ MPa} \leqslant P \leqslant 12.900 \text{ MIPa}\\ C_{pG} &= 0.1876175*\exp(0.2466925*P) \pm 5.00\\ &12.900 \text{ MPa} < P \leqslant 16.309 \text{ MIPa}\\ C_{pG} &= 7.620756E - 3*\exp(0.4117289*P) \pm 9.20\\ &16.309 \text{ MPa} < P < 18.743 \text{ MPa}\\ C_{pG} &= 6.5162612E - 6*\exp(0.7562i1*P) \pm 17.10\\ &18.743 \text{ MPa} \leqslant P < 20.40 \text{ MPa}. \end{split}$$

Dynamic viscosity, liquid phase at saturation

The following functions give an approximation to the dynamic viscosity of light water in the liquid phase, Visc_{L} [10⁻⁶ kg/m s], for saturation conditions. Their range of use is 0.035-21.45 MPa with the accuracy not worse than 0.10%. Figure 12 shows the accuracy of the approximation.

Approximation functions: = M.P.--s $Visc_1 = 111.5993 * P ** (-0.3425438) + 38.0$ 0.035 MPa ≤ P < 0.960 MPa $Visc_1 = 134.5288 * P **(-0.2843300) + 15.0$ **0.960** MPa $\leq P \leq 3.948$ MPa $Visc_1 = 141.5415 - 25.91353 * Im(P)$ 3.948 MPa < P < 9.514 MPa $V_{i5c_1} = 113.4599 * exp(-0.03279562 * P)$ $9.514 \text{ MPa} \le P < 15.074 \text{ MPa}$ $Visc_1 = 110.0 - 17.67922 * exp(0.05556056 * P)$ 15.074 MPa ≤ *P* < 18.868 MPa $Visc_{t} = 9.12152 * P - 0.3159837 * P * 2.0$ $18.868 \text{ MPa} \leq P < 20.430 \text{ MPa}$ $Visc_1 = 64.0 - 0.00261596 * exp(0.4010038 * P)$ 20.430 MPa $\leq P \leq$ 21.45 MPa. Dynamic viscosity, gas phase at saturation

The following functions give an approximation of the dynamic viscosity of light water in the gas phase. $Visc_G[10^{-6} \text{ kg/m s}]$, for saturation conditions. Their range of use is 0.040-21.35 MPa with the accuracy not worse than 0.065%. Figure 13 shows the accuracy of the approximation.

Approximation functions:

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 $V_{isc_{G}} = 7.473620 * P **(0.2050149) + 7.6$

0.040 MPa ≤ *P* ≤ **2.207** MPa

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Table 2. Summary of approximation functions					
Property	No. of functions	Range of use [MPa]	Worst accuracy [%]		
v _L	7	0.075-21.50	0.14		
D _G	7	0.085-21.50	0.22		
h_	6	0.075-21.70	0.10		
h _G	7	0.075-21.55	0.066		
Ū,	_	0.075-21.50	0.08		
$U_{\rm G}$		0.085-21.50	0.11		
Tui	5	0.070-21.85	0.02		
S _L	4	0.065-21.25	0.12		
s _G	5	0.025-21.50	0.10		
6	5	0.030-13.30	0.08		
CoL	3	13.30-20.30	0.60		
6	6	0.050-16.60	0.12		
CpG	3	16.00-20.40	0.60		
Visc	7	0.035-21.45	6.10		
Visc _G	6	0.040-21.35	0.065		

Table 2. Summary of approximation functions

 $Visc_{G} = 3.375163 * P **(0.3916208) + 11.8$

2.207 MPa < P ≤ 5.480 MPa

$$Visc_G = 0.9169410 * P * * (0.7644731) + 15.0$$

5.480 MPa < P < 9.585 MPa

 $Visc_{G} = 5.030544 * exp(0.5045239 * P) + 12.0$

 $9.585 \text{ MPa} \le P < 14.351 \text{ MPa}$

 $Visc_G = 0.4423761 * exp(0.1458726 * P) + 18.8$

 $14.351 \text{ MPa} \leq P < 81.385 \text{ MPa}$

 $V_{13c_G} = 0.01082229 * exp(0.3071918 * P) + 22.2$

18.385 MPa $\leq P \leq 20.347$ MPa

 $Visc_{G} = 6.6753655E - 6 * exp(0.6347700 * P) + 25.1$

 $20.347 \text{ MPa} < P \leq 21.35 \text{ MPa}.$

SUMMARY

The functions presented in this paper allow rapid calculation of the thermodynamic properties of light water for saturation conditions. Their range of use is from below 1b to just below the critical point with a high enough accuracy for the purpose of thermalhydraulic systems analysis. The ranges and accuracies for each property are summarized in table 2. It should be noted that internal energy, U, can be calculated using the correlations for specific volume and specific enthalpy and the equation U = H - PV. This yields an error of <0.11%.

Acknowledgements—Partial funding for this work was provided by the NSERC. The authors gratefully acknowledge the cooperation and contribution of the following: L. McKay (technician, McMaster University) and D. Klug (National Research Council of Canada).

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Property	No. of functions	Range of use [MPa]	Worst accuracy [%]
<i>v</i> _L	7	0.075-21.50	0.14
Ď _u	7	0.085-21.50	0.22
h_	6	0.075-21.70	0.10
h _G	7	0.075-21.55	0.066
$\tilde{U_{L}}$	_	0.075-21.50	0.08
U_{G}	_	0.085-21.50	0.11
T _{ut}	5	0.070-21.85	0.02
SL.	4	0.065-21.25	0.12
5 _G	5	0.025-21.50	0.10
-	5	0.030-13.30	0.08
$C_{p\perp}$	3	13.30-20.30	0.60
~	6	0.050-16.00	0.12
C_{pG}	3	16.00-20.40	0.60
Visc	7	0.035-21.45	0 10
Visc	6	0.040-21.35	0.065

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2.207 MPa $< P \le 5.480$ MPa

 $Visc_G = 0.9169410 * P ** (0.7644731) + 15.0$

5.480 MPa < P < 9.585 MPa

 $Visc_G = 5.030544 * exp(0.5045239 * P) + 12.0$

 $9.585 \text{ MPa} \leq P < 14.351 \text{ MPa}$

 $Visc_{G} = 0.4423761 * exp(0.1458726 * P) + 18.8$

 $14.351 \text{ MPa} \leq P < 81.385 \text{ MPa}$

 $Visc_{G} = 0.01082229 * exp(0.3071918 * P) + 22.2$

 $18.385 \text{ MPa} \leq P \leq 20.347 \text{ MPa}$

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The functions presented in this paper allow rapid calculation of the thermodynamic properties of light water for saturation conditions. Their range of use is from below 1b to just below the critical point with a high enough accuracy for the purpose of thermalhydraulic systems analysis. The ranges and accuracies for each property are summarized in table 2. It should be noted that internal energy, U, can be calculated using the correlations for specific volume and specific enthalpy and the equation U = H - PV. This yields an error of <0.11%.

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APPENDIX

The Rate Form of the Equation of State

The development of a non-iterative equation of state for two-phase flow systems was recently investigated (Sollychin *et al.* 1985; Garland & Sollychin 1988). At present, the equation of state is usually solved by iterative numerical techniques. By recasting the equation of state the time derivative of P can be solved directly and the use of iterative methods can be eliminated. The time derivative form of the equation of state was developed by considering an arbitrary volume of two-phase fluid as a thermodynamic system where both phases are at saturation under a uniform saturation pressure, P. By utilizing the total mass of the fluid, M, the total enthalpy in the system. H, the volume of the system, V, and taking the derivatives of these quantities with respect to time, one obtains [A.1] which is dependent on the initial pressure and on the rate of change of mass, volume and enthalpy in the system:

$$\frac{dP}{dt} = \frac{F_1(P)\frac{dM}{dt} + F_2(P)\frac{dH}{dt} + F_3(P)\frac{dV}{dt}}{M_gF_4(P) + M_fF_5(P)},$$
[A.1]

where

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$$F_{1}(P) = h_{G} * v_{L} - h_{L} * v_{G},$$

$$F_{2}(P) = v_{G} - v_{L},$$

$$F_{3}(P) = -(h_{G} - h_{L}),$$

$$F_{4}(P) = \frac{dh_{G}}{dP}(v_{G} - v_{L}) - \frac{dv_{G}}{dP}(h_{G} - h_{L})$$

and

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$$F_{\rm S}(P) = \frac{\mathrm{d}h_{\rm L}}{\mathrm{d}P}(v_{\rm G} - v_{\rm L}) - \frac{\mathrm{d}v_{\rm L}}{\mathrm{d}P}(h_{\rm G} - h_{\rm L}).$$

This form involves combinations of the saturation values of specific volume and specific enthalpy in liquid and gas phases, and the derivatives of these properties with respect to pressure. Thus we can incorporate the approximation functions described above to easily solve the equation of state [1]. The derivatives are determined simply by taking the derivatives of the approximation functions with respect to pressure.

Sec. 1