STEAMEST: A Software Tool for Estimation of Physical Properties of Water and Steam

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***Abstract*—A software tool, STEAMEST, has been developed for estimation of properties of water and steam for industrial applications using IAPWS-IF97 industrial formulation and subsequent updates. STEAMEST meets the precision and consistency standards of the International Association for the Properties of Water and Steam (IAPWS) as verified by 8 byte real values for all variables. It achieves maximum conformity (a tolerance of 1 part per billion) with "Basic Equations" of IAPWS-IF97 through use of iterative procedures instead of approximate "Backward Equations", where recommended "Basic Equations" are not available. The code has been written in highly flexible Microsoft .NET framework using an object-oriented approach to ensure portability and modularity in software design without making any compromise on performance. Given valid input(s), STEAMEST can predict more than 15 properties of water/steam with a user-selected precision. It includes integrated software for unit conversion. Thermodynamic plots created by STEAMEST have the provision of zooming a specified portion.**

STEAMEST can compete with similar software both in terms of performance and reliability. Thus it has the potential to become a valuable tool for industry and academia.

***Index Terms*—software tool, properties of water and steam, IAPWS-IF97, STEAMEST**

I. Introduction

Ordinary water substance (H_2O) is the single most frequently used material in the process industry. Precise estimation of properties of water and steam has always been a challenging task. A lot of research has focused on estimating these properties and numerous tabular and mathematical formulations have been devised over the years for this purpose.

The International Association for the Properties of Water and Steam (IAPWS) is an international non-profit association of national organizations concerned with the properties of water and steam, particularly thermo-physical properties and other aspects of high-temperature steam, water and aqueous mixtures that are relevant to thermal power cycles and other industrial applications. IAPWS provides internationally accepted formulations for the properties of light and heavy steam, water and selected aqueous solutions for scientific and industrial applications. It also defines the research needs and promotes and coordinates research on such systems [1].

Efforts to produce international agreement on values for the properties of water and steam began with International Steam-Table Conferences (held in 1929, 1930, and 1934). The first internationally accepted formulation was a set of "Skeleton Tables" in 1934. These were later revised in 1963, 1985, and in 1994 to reflect the new state of knowledge about the subject. The last skeleton tables were withdrawn by IAPWS in 2003, and now the IAPWS recommendations are exclusively equation-based [2].

With the advent of high-speed computers and their wide-spread use in industry as well as in personal computing, the focus has gradually shifted to the use of equation-based formulations. A preliminary formulation IFC-66 for industrial use was adopted in 1966 on the basis of 1963 Skeleton Tables. The same was subsequently revised as IFC-67 in 1967. IFC-67 became obsolete with the adoption of the IAPWS-IF97 formulation for industrial use in 1997. Literature references for these and many other formulations may be found in [2].

The choice of a particular formulation from a set of possible alternatives is dictated by the precision requirements in property estimation and the time available for computation of results. High-speed computers have made it possible to solve more complex relationships within fractions of a second with better precision.

II. Background

The most accurate state-of-the-art formulation recommended by IAPWS for estimation of thermodynamic properties of water is the "IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use", IAPWS-95 [3]. This formulation provides a basic equation for the specific Helmholtz free energy as a function of temperature and density. The dimensionless

specific Helmholtz energy is determined in two components, i.e., ideal-gas part and the residual part.

$$\frac{f(\rho,T)}{RT} = \phi(\sigma,\tau) = \phi^o(\sigma,\tau) + \phi^r(\sigma,\tau) \qquad (1)$$

Where **σ** and **τ** are respectively dimensionless density and dimensionless temperature. These ideal and residual parts of dimensionless specific Helmholtz energy are calculated using tabulated values of coefficients and exponents with the equations provided. Equations have also been provided for estimation of other thermodynamic properties using the ideal and residual parts of dimensionless specific Helmholtz energy and their derivatives [3].

Although IAPWS-95 is recommended for general and scientific use, the calculations are tedious and time-consuming. The properties of water and steam are usually required at some known temperature and pressure. This does not conform to the structure of (1). Hence an iterative solution of Maxwell's phase equilibrium conditions is required. The problem is further complicated by the existence of two solutions below critical point (one for saturated liquid and the other for saturated vapor) [4]. For design simulations involving water and steam, these correlations often need to be called millions of times leading to increased calculation time. This limitation suggests that a special formulation may be developed for accelerated computation, even if the user has to compromise on the precision of results to some extent. For this purpose, IAPWS has developed a separate formulation called "IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam", IAPWS-IF97 [4]. The equations provided in IAPWS-IF97 are applicable for the following ranges:

$$\begin{aligned} &273.15K \le T \le 1073.15K, \quad p \le 100MPa \\ &1073.15K \le T \le 2273.15K, \quad p \le 50MPa \end{aligned} \qquad (2)$$

The entire range of validity of IAPWS-IF97 is divided in 5 regions (see Fig. 1). Regions 1, 2 and 5 are covered by fundamental equations for specific Gibbs free energy ***g (p, T)***. Region 3 is covered by a fundamental equation for specific Helmholtz free energy ***f (ρ, T)***. Region 4, representing the saturation curve, is covered by saturation-pressure equation p_s ***(T)***. These basic equations yield corresponding values from IAPWS-95 within the tolerance limits specified for the development of corresponding equations [4]. All other thermodynamic properties in a particular region can be calculated using derivatives and similar functions of the corresponding basic equation.

When the input data is not available for use in basic equations, IAPWS-IF97 and several subsequent releases provide so-called "backward equations" to avoid iterative calculations of main parameters. The numerical consistencies of these backward equations with the basic equations of IAPWS-IF97 are usually sufficient for heat cycle and steam turbine calculations. However, when the demands on the numerical consistencies are extremely high, e.g., where further calculations are to be based on the estimations obtained by use of backward equations, iterations using IAPWS-IF97 basic equations are necessary [5-8].

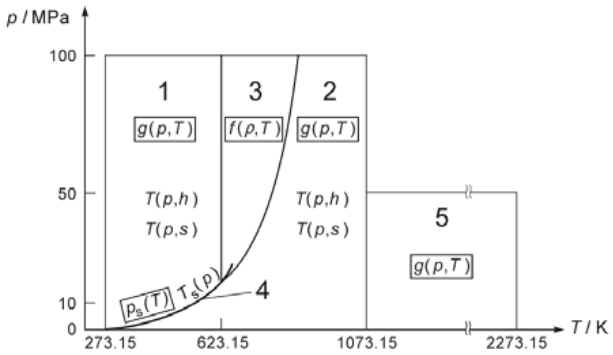

Figure 1. The 5 regions of IAPWS-IF97. Functions within boxes show basic equations for the corresponding regions. Other functions in regions 1 and 2 represent backward equations. Adopted from IAPWS-IF97 [4].

The consistency standard of IAPWS can be understood from Fig. 1. In region 1, one basic equation ***g (p, T)*** and two backward equations ***T (p, h)*** and ***T (p, s)*** are shown. If the use of basic equation is required, the input parameters are ***p*** and ***T***. However, if the available information is in the form of ***p*** and ***h***, then first ***T*** will need to be calculated using the respective backward equation. Since backward equations provide an estimate, therefore this calculated value of ***T*** will need to be verified according to the IAPWS consistency standard. For this, ***h*** will be calculated using a derivative of the basic equation. The consistency requirements are satisfied if the user-specified and calculated values of ***h*** do not show any difference when using 8-byte real variables.

A number of software products have been developed using IAPWS-IF97, e.g., NIST/ASME Steam Properties Database [9], StmProps [10], WSProps [11], XSteam [12], and the software by Dr. Wagner [13]. These software products implement the previous versions of the IAPWS-IF97 formulation, and do not include the latest revisions that might result in increased range of applicability and significantly improved precision. For example, the original formulation released in 1997 covered pressures up to 10 MPa in region 5. With the latest revision in 2007, this range has been extended up to 50 MPa. In order to incorporate these revisions in formulation, an update to the existing software or new software is required.

III. STEAMEST

STEAMEST[1] has been developed using the latest revision of IAPWS-IF97 formulation. STEAMEST offers high precision calculations for estimation of properties without excessive CPU-time requirements. The software code is object-oriented that is fully compatible with

[1] STEAMEST is free for educational purposes and can be downloaded from http://www.uet.edu.pk

existing and future versions of the Microsoft Windows[2] operating system.

A. GUI and Algorithm

Fig. 2 presents a screenshot of the Microsoft Windows-compatible interface developed for STEAMEST using Microsoft Visual Basic .NET 2005 Express Edition. This choice of programming language has made it possible to develop a clear and manageable object-oriented code that is portable on any system running .NET Framework version 2.0 or later. The .NET language compilers give output in the form of MSIL (Microsoft Intermediate Language). This output is then converted to native code by JIT (just-in-time) compilers, and the native code is then run by CLR (Common Language Runtime). This choice ensures that the code of the program can be written in any programming language supported by .NET framework. Additional modules can be added to expand the functionality of the software with little effort. CLR also takes cares of the memory management and minimizes the possibility of a memory leak in the system. This results in high performance with little memory requirements. An added advantage is the flexibility to produce different software products with minor changes in code, e.g., function libraries that can become parts of other software packages, Microsoft Excel[3] add-in, or a distributed application using a web interface.

The self-explanatory GUI of STEAMEST makes it easy to use even for a novice user. The user can choose a pre-customized set of units for the results, and a desired level of precision. Each parameter has an associated dropdown list of units that the user can use to further modify the choice of units. An integrated unit converter makes it possible to view the results in a number of commonly used units for each parameter. The interface is designed in such a way that any change of selection by the user is immediately propagated in both upward and downward directions of software workflow resulting in necessary updating of the output.

The algorithm of STEAMEST is presented in Fig. 2. In the very first step, the user input is validated against non-numeric entries and out-of-range numeric entries that can cause the solver to crash. Then depending upon the selected input parameter(s), the software calls the appropriate functions as outlined in Table 1. After determination of the corresponding IAPWS-IF97 region, the software checks whether single-phase or two-phase properties need to calculated, and enables/disables corresponding elements of the results page. If the input combination conforms to the basic equation for the region under consideration, the calculations are directly based on the equations provided in IAPWS-IF97. Otherwise, a suitable backward equation is chosen to make a good initial guess for the iteration. One-dimensional iterative calculations are carried out within a range of the initial

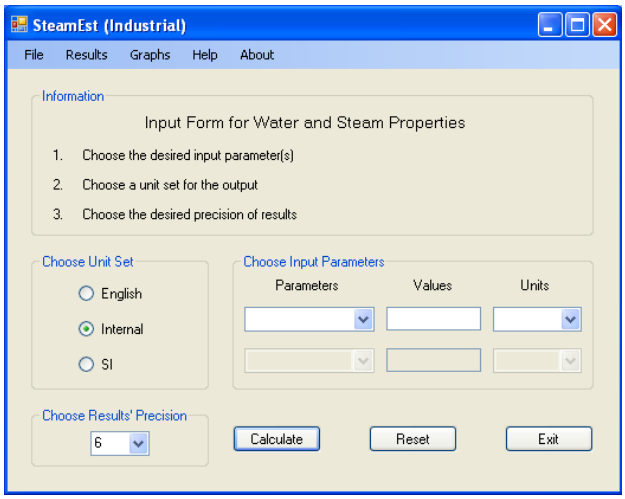

Figure 2. GUI of STEAMEST

guess using the corresponding basic equation to meet the recommended consistency standards.

When the absolute difference between the values of selected iterative parameter in two successive iterations is less than one part per billion, iterations converge. Such a high level of conformity with the corresponding basic equation ensures that the results can be further utilized for determination of the remaining parameters using basic equation. Because of good initial guesses and a relatively small search domain for the precise solution, this level of

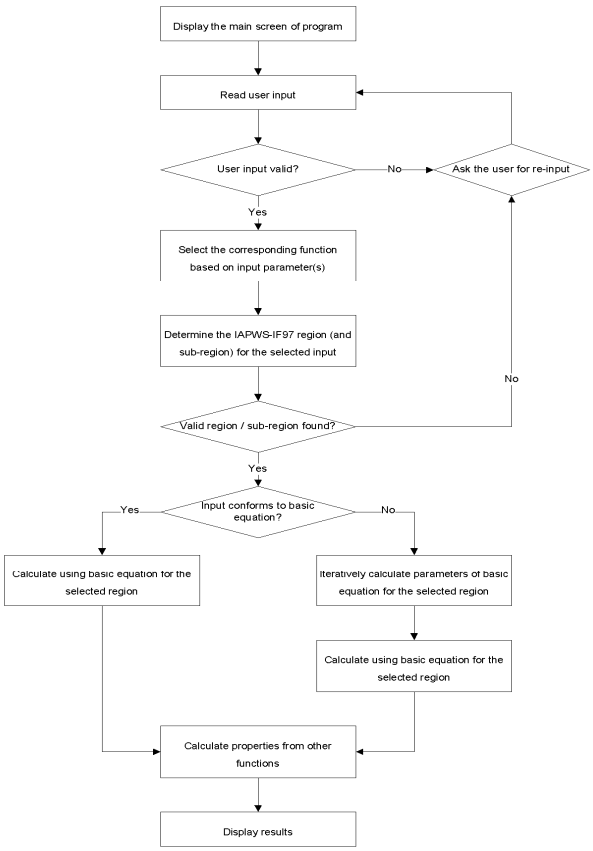

Figure 3. Working algorithm of STEAMEST

[2] Windows is a registered trademark of Microsoft Corporation. http://www.microsoft.com

[3] Excel is a registered trademark of Microsoft Corporation. http://www.microsoft.com

TABLE 1.
ACCEPTED INPUT(S) AND CORRESPONDING CALCULATION PROCEDURES

Set	Input	Region	Functions for Calculation
1	P or T	4	Saturation pressure/temperature equation. Then basic equations of regions 1, 2, or 3 at corresponding region boundaries with region 4.
2	P & x or T & x	4	Same as in Set 1. Then calculations inside 2-phase region using definition of vapor fraction.
3	P & T	1, 2, 5	IAPWS-IF97 basic equation for the corresponding region.
		3	Iteration of IAPWS-IF97 basic equation for region 3 using a suitable backward equation for unknown *v*. Then IAPWS-IF97 basic equation for region 3.
4	P & H or P & S or T & H or T & S	1, 2, 5	Iteration of IAPWS-IF97 basic equation for the corresponding region for unknown P or T. Then same as in Set 3.
		3	Iteration of IAPWS-IF97 basic equation for region 3 using a suitable backward equation for unknown P or T. Then same as in Set 3.
		4	Same as in Set 1. Then calculations inside 2-phase region using definition of vapor fraction.
5	H & x or S & x	4	Iteration using IAPWS-IF97 basic equations for regions 1, 2, and 3 at region boundaries for unknown P. Then same as in Set 2.
6	H & S	1, 2, 3	Backward equations for the corresponding region for unknown P. Then same as in Set 4.
		4	Backward equation for T_{sat} in region 4. Then same as in Set 4.

convergence is usually achieved in less than 20 iterations without consuming excessive CPU-time. After the iterations have converged, the remaining calculations proceed with the use of corresponding basic equation.

B. Graphing Capabilities

Besides providing numerical results, STEAMEST has the capability to produce some of the most commonly used graphs of thermodynamic parameters for ordinary water substance. It uses the open source graphics library ZedGraph to provide several advantages, e.g., printing, copying and pasting to other Windows compatible applications, and exporting as images in six different standard graphics formats [14]. It also provides support for using the mouse to zoom in or out in order to view fine details of the curve behavior in any valid region. Another special feature is displaying the coordinates of a point when the mouse hovers over it. These capabilities have been illustrated in screenshots presented in Fig. 4(a) and 4(b).

IV. CASE STUDIES

Two case studies are presented, as per Set 1 and 3 of Table 1, to demonstrate the working of the software by outlining the respective calculation procedure for each case.

A. Input: p = 2 bar

The calculations for this particular case follow Set 1 of Table 1. Since only a single input parameter is there, the point of interest lies on the boundary of two-phase region, and the resulting phase may be a saturated liquid or saturated vapor. The necessary steps of calculations for this case are listed below.

1. Input pressure value is converted to required internal working unit (MPa).
2. Using the saturation-temperature equation, calculate the corresponding saturation

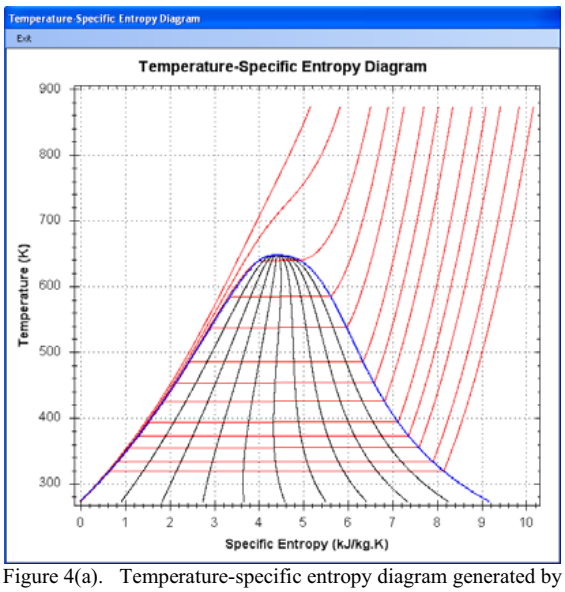

Figure 4(a). Temperature-specific entropy diagram generated by STEAMEST for temperature range of triple point to 873.15 K (600 °C)

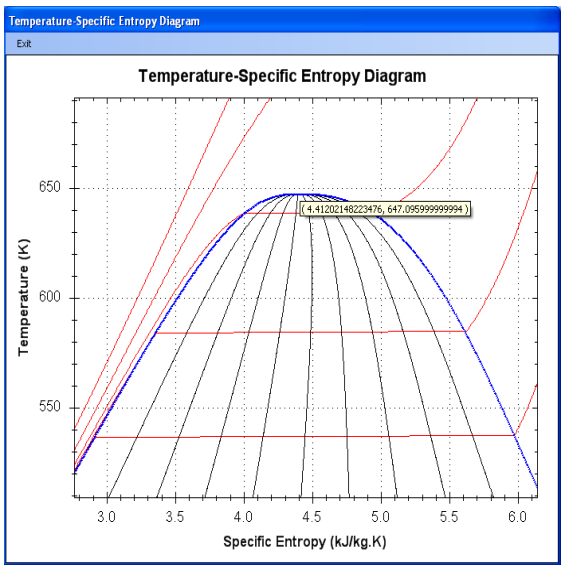

Figure 4(b). Temperature-specific entropy diagram focused near the critical point. The coordinates of the critical point are visible.

temperature. This is evaluated as approximately 393.36 K.

3. The saturation temperature is less than the upper temperature limit of region 1 of IAPWS-IF97, which is 623.15 K. Therefore, the point of interest lies on the boundary between regions 1 and 4 (saturated liquid) or on the boundary between regions 2 and 4 (saturated vapor).
4. The properties for saturated liquid h^L, s^L, u^L, v^L, cp^L, cv^L, *and* w^L are calculated using basic equation of region 1 for the point (p_{input}, T_{sat}).
5. The properties for saturated vapor h^V, s^V, u^V, v^V, c_p^V, c_v^V, *and* w^V are calculated using basic equation of region 2 for the point (p_{input}, T_{sat}).
6. MV^L, ρ^L, MV^V, *and* ρ^V are calculated using v^L and v^V.
7. μ^L *and* μ^V are calculated using the recommended interpolating equation of "IAPWS Revised Release on the IAPS Formulation 1985 for the Viscosity of Ordinary Water Substance" [15].
8. k^L *and* k^V are calculated using the recommended equation of "IAPWS Revised Release on the IAPS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substance" [16].
9. Pr^L, Pr^V, v^L, *and* v^V are calculated from their definition.
10. VP is calculated using the recommended equation of "IAPWS Revised Supplementary Release on Saturation Properties of Ordinary Water Substance" [17].
11. σ is calculated using the recommended equation of "IAPWS Release on Surface Tension of Ordinary Water Substance" [18].

The results for saturated liquid and saturated vapor are respectively shown in screenshots presented in Figures 5(a) and 5(b).

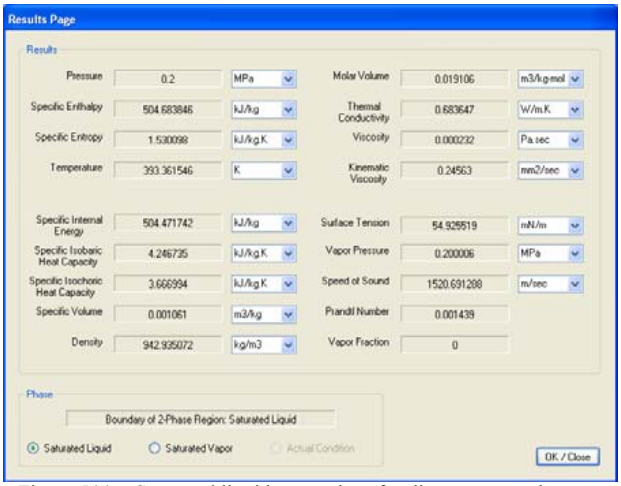

Figure 5(a). Saturated liquid properties of ordinary water substance *(p = 2 MPa)*

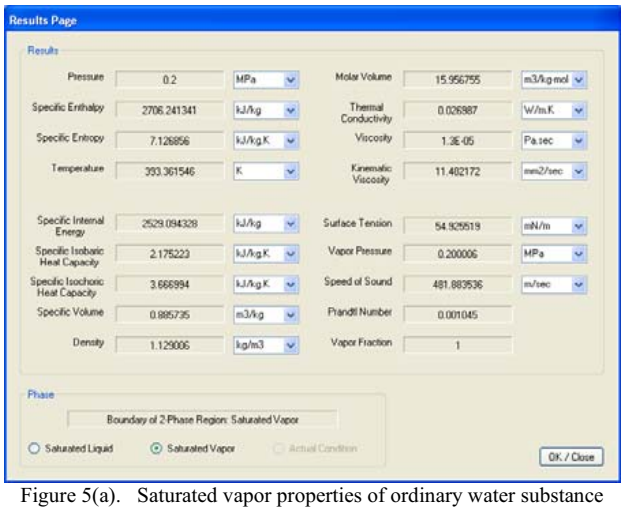

Figure 5(a). Saturated vapor properties of ordinary water substance *(p = 2 MPa)*

B. Input: p = 50 MPa, T = 630 K

The calculations for this particular case follow Set 3 of Table 1. The first step is to locate the region in which the point of interest lies. As indicated by the region boundaries in Fig. 1, this particular state point is located in region 3. However, the basic equation for region 3 is in the form $f(\rho, T)$. Hence either we have to use the backward equations, or an iterative procedure. The steps carried out by STEAMEST for the calculations are outlined below. The results are shown in Figure 6.

1. Using the IAPWS release on backward equations for specific volume in region 3 as a function of temperature and pressure, the point of interest in found to be located in sub-region 3a [8]. Using the corresponding backward equation, an initial value of v is determined.
2. The precise value of v is assumed to be within ±2% of the initial guess. Bisection method is

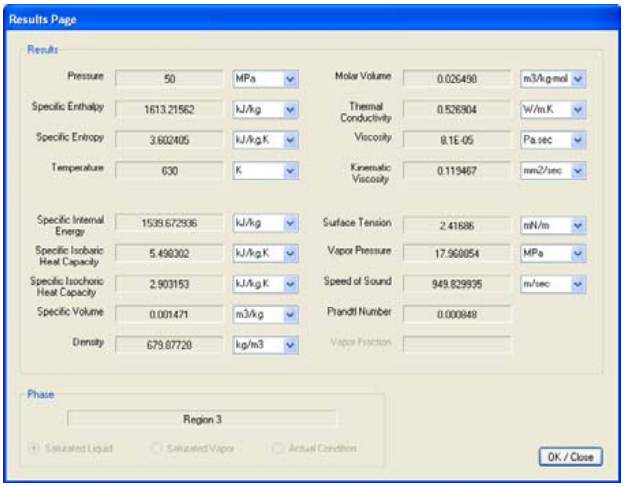

Figure 6. Properties of ordinary water substance *(p = 50 MPa and T = 630 K)*

used within these limits for iteration of basic equation for region 3. The converged calculations can be used to yield a precise value of ρ that is in complete agreement with the given value of pressure.

3. This state point represents a single phase; therefore the remaining calculations are made for the single phase following the steps outlined in for first case study A.

V. Conclusions

STEAMEST is a tool for calculations of various properties of ordinary water substance using IAPWS-IF97 and subsequent updates. The software is user-friendly and offers accelerated calculations with controllable precision. It ensures protection against invalid user inputs and runtime errors. It includes an integrated unit converter and has powerful graphing capabilities. This tool is expected to be of significant importance for industrial as well as educational purposes. Graphical representations of interdependence of various parameters help better understanding their relationships. STEAMEST can compete with similar software products in terms of performance, precision, and portability. A modular approach in programming has led to its versatility and flexibility of re-using some segments or the entire code in several manners. It may be used to create function libraries that can become part of other simulation tools, or for development of a web interface for distributed computing of properties of water and steam.

Nomenclature

A. Symbols

c_p	Specific isobaric heat capacity
c_v	specific isochoric heat capacity
f	Specific Helmholtz free energy
g	Specific Gibbs free energy
h	Specific enthalpy
k	Thermal conductivity
MV	Molar volume
p	Pressure
Pr	Prandtl number
s	Specific entropy
T	Temperature
u	Specific internal energy
v	Specific volume
VP	Vapor pressure
w	Speed of sound

B. Superscripts

L	Saturated liquid phase
V	Saturated vapor phase

C. Greek letters

μ	Dynamic viscosity
ρ	Density
σ	Surface tension
υ	Kinematic viscosity

References

[1] Website reference: http://www.iapws.org

[2] Web document reference: http://www.iapws.org/relguide/Obsolete.pdf

[3] IAPWS Release on the *IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use*, September 1996. Available at http://www.iapws.org

[4] IAPWS Revised Release on the *IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam*, August 2007. Available at http://www.iapws.org

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[6] IAPWS Revised Supplementary Release on *Backward Equations for the Functions T (p, h), v (p, h) and T (p, s), v (p, s) for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam*, September 2004. Available at http://www.iapws.org

[7] IAPWS Supplementary Release on *Backward Equations p (h, s) for Region 3, Equations as a Function of h and s for the Region Boundaries, and an Equation T_{sat} (h, s) for Region 4 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam*, September 2004. Available at http://www.iapws.org

[8] IAPWS Supplementary Release on *Backward Equations for Specific Volume as a Function of Pressure and Temperature v (p, T) for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam*, July 2005. Available at http://www.iapws.org

[9] Website reference: http://www.NIST.gov

[10] Website reference: http://www.gpengineeringsoft.com

[11] Website reference: http://www.sourceforge.net/projects/innohex

[12] Website reference: http://www.x-eng.com

[13] Website reference: http://www.ruhr-uni-bochum.de

[14] Website reference: http://www.sourceforge.net/projects/zedgraph

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[16] IAPWS Revised Release on the IAPS Formulation 1985 for the *Thermal Conductivity of Ordinary Water Substance*, September 1998. Available at http://www.iapws.org

[17] IAPWS Revised Supplementary Release on *Saturation Properties of Ordinary Water Substance*, September 1992. Available at http://www.iapws.org

[18] IAPWS Release on *Surface Tension of Ordinary Water Substance*, September 1994. Available at http://www.iapws.org