

A Web Service for Thermodynamic Properties of Pure Water Based on P-T Computational Scheme of IAPWS-95 and IAPWS-IF97 formulations

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ABSTRACT

A web service, <http://www.INEELGeoSteam.NET/INEELSteamTables.aspx> is developed for the thermodynamic properties of pure water. It uses the SOAP (Simple Object Access Protocol) and is based on the assembly, *INEEL.ThermoData.Wtr.dll* written in Visual Basic in Visual Studio. The web service calculates 23 properties as function of temperature (T) and pressure (P) using the IAPWS-95 scientific and IAPWS-IF97 industrial formulations. The interoperability (i.e., independent of programming language, operating system and platform software) of the web service is illustrated by its use in Excel (i.e., in COM- Component Object Model), in C# (i.e., .NET framework) and a water-heating application in windows platform. It shows that the fluid region is made of compressed liquid and superheated steam and the critical isochor is the separation boundary between them. The water heating vessel program will be extended in future for geochemical model of geothermal reservoir.

1. INTRODUCTION

The development of computer programming progressed through various phases of resolving the deficiencies of existing technology: *structured programming, object-oriented programming, distributed computing, electronic data interchange, World Wide Web, and Web services* (W3C, 2004). A web service is a software system designed to interact or invoke a method directly with other applications over the internet using open standards and protocols like HTTP (Hyper Text Transfer Protocol), XML (Extensible Markup Language) and SOAP (Simple Object Access Protocol). The web services are interoperable; so, a web service built on a platform can be consumed in any other application on any platform (Kudithipudi, 2012).

Thermodynamic properties of water (i.e., steam tables) are essential in understanding the origin and mechanisms of natural physical, chemical, geological and biological processes in the earth's atmosphere, surface and crust (Tang, 2016). In the electricity industry, water vapor (steam) is a working fluid of electricity generation power plants (Soo, 1968; Taylor, 1983). The steam tables play a vital role in calculating the efficiency and numerical simulation of steam transport in these plants (Verma, 2013). In geothermal power plants, the steam separated at the wellhead of a production well is transported to the turbine through a pipeline network, which consists of tubes, elbows, Tees, valves, expansions, reductions, etc. The pressure (P), temperature (T) and flow-rate (Q) in the geothermal wells depend on the natural characteristics of the geothermal reservoir; therefore, the steam transport is influenced by the topography and the location of geothermal wells and power plants (García et al., 2009). Similarly, the thermodynamic database of chemical species and minerals including the steam tables is a basis for the geochemical modelling of aquatic systems (Nordstrom et al., 1979; Torre-Alvarado et al., 2012). Thus, the steam tables of pure water are fundamental to many engineering and scientific studies.

Initially, the data tables of experimental values of thermodynamic properties of water were programmed in computer codes; however, updating and maintaining these tables were difficult tasks (Span, 2000). Therefore, the experimental thermodynamic datasets were fitted in empirical relations, known as the equation of state or formulation (Wagner and Pruß, 2002; Verma, 2003). The fundamental works in developing the formulation for a wide range of temperature and pressure are from Keenan et al. (1968), Irvine and Liley (1984), Haar et al. (1984), Hill (1990) and Wagner and Pruß (2002). Wagner and Pruß (2002) presented a comprehensive study on the evolution of these thermodynamic formulations for the properties of pure water from the first formulation (*IFC-68*) to the most accepted *IAPWS-95* formulation. Presently, the p-T computation schemes: *IAPWS-95 for scientific use* Wagner and Pruß (2002) and *IAPWS-IF97 for industrial use* (IAPWS, 2007) are widely accepted. The accuracy, computing speed and numerical consistency in the tabulated thermodynamic properties of water through the formulations is the subject of recent studies (Verma, 2011; Wang et al., 2012). There is still a requirement of higher computation speed for the thermodynamic properties of water for real-time simulation of steam transport problems like designing the steam power plant (Wang et al., 2012) and transporting steam from geothermal wells to the geothermal power plant (Verma, 2011). Verma (2011) developed a linear interpolation scheme on the P-T surface grid to accelerate the calculation of the thermodynamic properties of water using the *IAPWS-95* formulation. Similarly, Wang et al. (2012) presented a spline interpolation scheme on the P-T surface grid for the calculation of the thermodynamic properties of water using the *IAPWS-IF97* formulation. Verma (2016) studied a comparative evaluation of both *IAPWS-95* and *IAPWS-IF97* formulations for computational speed and accuracy in the calculated properties. The execution time for *IAPWS-IF97* is generally 70 times less than that of *IAPWS-95*. The P-T precision for both formulations is within $T=\pm 0.1$ K and $P=\pm 0.001$ MPa.

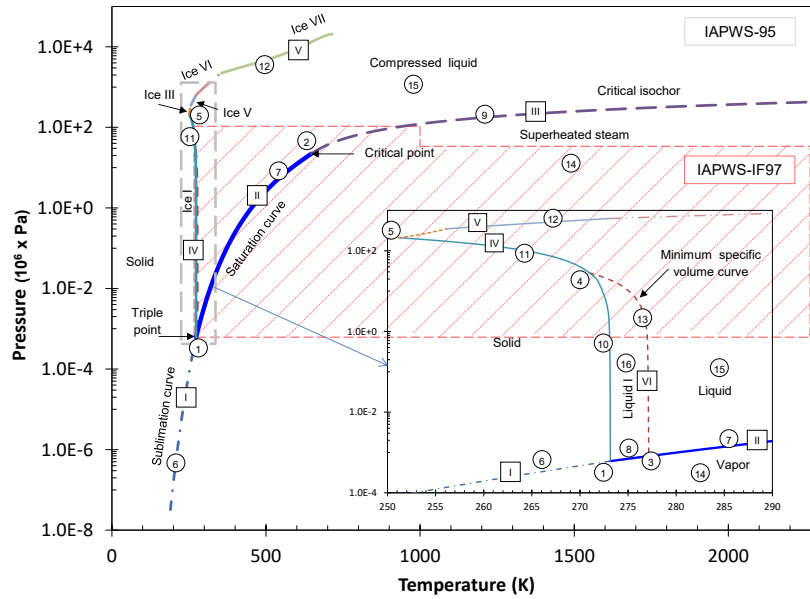


Figure 1: p-T phase diagram of pure water, according to the IAPWS-95 formulation. The sixteen states are marked with a number in a circle (1-5 as triple points, 6-13 as separation boundaries and 14-16 as phase regions) and six separation boundaries are marked as a roman number I to VI in a rectangle. The inserted figure is an amplification to illustrate the triple points. The shaded area with the dashed diagonal line represents the region of validation for the IAPWS-IF97 formulation.

For the IAPWS-95 and IAPWS-IF97 formulations, the dynamic link libraries (DLL) or assembly were written to get the reusability of steam tables of pure water in different programs (Span, 2000; Wagner and Pruß, 2002; Verma, 2003, 2016). Similarly, there are various commercial and scientific applications to tabulate the steam tables of pure water (Wagner and Pruß, 2002; Verma, 2003; Wang et al., 2012); however, the present demand of computer programming world is interoperability (i.e., independent of programming language, operating system and platform software), which is obtained by creating the web services (W3C, 2004; Kudithipudi, 2007).

The paper presents the development of a web service, <http://www.INEELGeoSteam.NET/INEELSteamTables.aspx>, for the thermodynamic properties of pure water, which is based on the updated assembly, INEEL.ThermoData.Wtr (Verma, 2016). The interoperability of the web service is illustrated as demo applications to tabulate the steam tables in C# and Excel and water heating application on the Windows platform.

2. P-T PHASE DIAGRAM OF IAPWS-95 AND IAPWS-IF97 FORMULATIONS

Figure 1 shows the P-T surface of pure water for the IAPWS-95 formulation. There are six separation boundaries, which are marked with a Roman numeral, I to VI, in a rectangle. The boundaries are named as *Sublimation*, *Saturation*, *CriticalIsochor*, *IceMelting*, *IceIII_VIIMelting*, *MinimumVolume*, respectively. Along the separation boundaries, there is only one independent variable, either T or P. Similarly, there are 16 water states, which are marked with a number in a circle (1-5 as fixed points (four triple points and a critical point), 6-13 as separation boundaries and 14-16 as phase regions). The states are *TriplePoint*, *CriticalPoint*, *MinimumVolumeSaturationPoint*, *IceI_Liquid_LiquidIPoint*, *IceI_IceIIIPoint*, *Sublimation*, *SaturationLiquid_Vapor*, *SaturationLiquidI_Vapor*, *CriticalIsochor*, *IceI_LiquidCurve*, *IceI_LiquidI_Curve*, *IceIII_IceVIIMeltingCurve*, *MinimumVolumeCurve*, *SuperheatedSteam*, *CompressedLiquid*, *CompressedLiquidI*, respectively. The shaded area with dashed diagonal lines in Figure 1 shows the region of validation of the IAPWS-IF97 formulation.

Figure 2 shows the P-T surface of pure water for the IAPWS-IF97 formulation. The P-T region covered by the IAPWS-IF97 formulation is generally sufficient for the study of systems in engineering and natural sciences; however, the IAPWS-IF97 formulation does not calculate all the properties. It is divided into five regions and each region has a different set of equations for the thermodynamic properties (IAPWS, 2007). The division of liquid phase into “liquid” and “liquid I” by the minimum volume curve is not considered in the IAPWS-IF97 formulation (Verma, 2009). The critical Isochor represents the continuous transformation boundary between the liquid and vapor phases.

3. WEB SERVICE FOR STEAM TABLES OF PURE WATER

The web service, INEELSteamTables.aspx is based on the assembly, INEEL.ThermoData.Wtr.dll and is hosted on the URL address <http://www.INEELGeoSteam.NET/INEELSteamTables.aspx>. A brief description of each method is included in the web service. There are three methods for each IAPWS95 and IAPWS-IF97 formulations. The methods calculate the water properties as a function of (1) T and (2) P along the separation boundaries and (3) T and P at any point on the P-T surface, respectively. Similarly, there are two methods to study the behavior of water heating in a closed container, written using the IAPWS95 formulation. Additionally, six methods in the web service, corresponding classes *MKSSteamTables95* and *MKSSteamTablesIF97* in the assembly INEEL.ThermoData.Wtr.dll, are programmed to standardize the MKS measurement units of input and output parameters for the respective formulation.

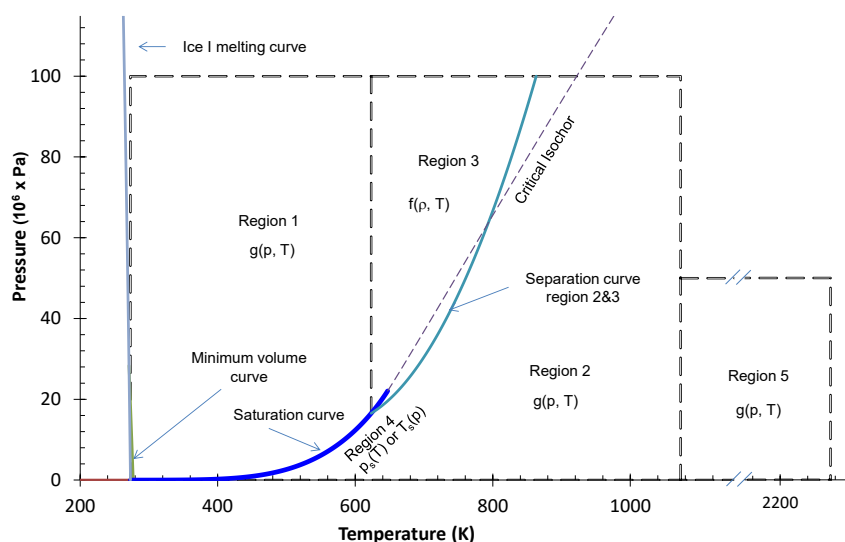


Figure 2: p-T phase diagram of pure water considered in the IAPWS-IF97 formulation, divided in five regions (IAPWS, 2007). Each region has different set of equations for the thermodynamic properties. The division of liquid phase into liquid and liquid I by the minimum volume curve is not considered in this formulation. The critical Isochor represents the continuous transformation boundary between liquid and vapor phase.

To test the web service <http://www.INEELGeoSteam.NET/INEELSteamTables.aspx>, type the URL in a browser and press return. It shows the list of links to all the methods of web service. Let us click on the method, MKSIAPWS95TP. It shows the input parameter list of the method. If we type the value of Temp (temperature in K) as 500 and Press (pressure in Pa) as 3000000, it displays the water properties in the XML format. The measurement units of all the calculated parameters are the MKS system. For the condition of T and P, the water phase is the compressed liquid and vapor properties are displayed as -1 (i.e., no vapor phase).

Now, we will explain the use of steam tables web service in different environments and the computer-code is available from the author to assist users to implement the steam tables in their applications.

3.1 Using the Web Service in Excel

The development of Excel is based on the Component Object Model (COM). The procedure for calling a web service in an Excel function (DontFredBrett, 2010) is the following

- Install the Microsoft Internet Explorer.
- Activate the “Developer” tab in Excel.
- Open the Visual Basic window and add reference to the libraries, *Microsoft Internet Controls* and *Microsoft HTML object library*, in the Tools tab.
- The code for excel functions is given in a file as the electronic supplementary material (Excel.txt). Copy the code in a module in the personal workbook, Personal.xlsb. A function written in the personal workbook is available in all the workbooks (Verma, 2003). The IAPWS95 formulation is only used here; but the similar code can be written for the IAPWS-IF97 formulation.

There are five functions: *TSep*, *PSep*, *WtrStmTbl95T*, *WtrStmTbl95P*, and *WtrStmTbl95TP*. The use of these functions is similar as documented by Verma (2003); but the web service is used here and the steam tables properties are in MKS units. For example, there are four input parameters for the function *WtrStmTbl95TP*: temperature (in K) =500, pressure (in Pa) = 3000000, phase no. (1- Liquid, 2- Vapor) =1, and property no. (23 properties listed in Figure 2c) = 5. The function calculates the value of liquid enthalpy (in kJ/kg) = 975.508.

3.2 Tabulation of Steam Tables in a Windows Form Application

The procedure for consuming a web service in a Windows form application in the Visual Studio is the following

- Create an empty Windows application, StmTblApp in C#.
- Add a reference to the web service, <http://www.INEELGeoSteam.NET/INEELSteamTables.aspx>.
- Add a Windows form, named as frmMain.aspx.
- Add the controls as shown in Figure 4.

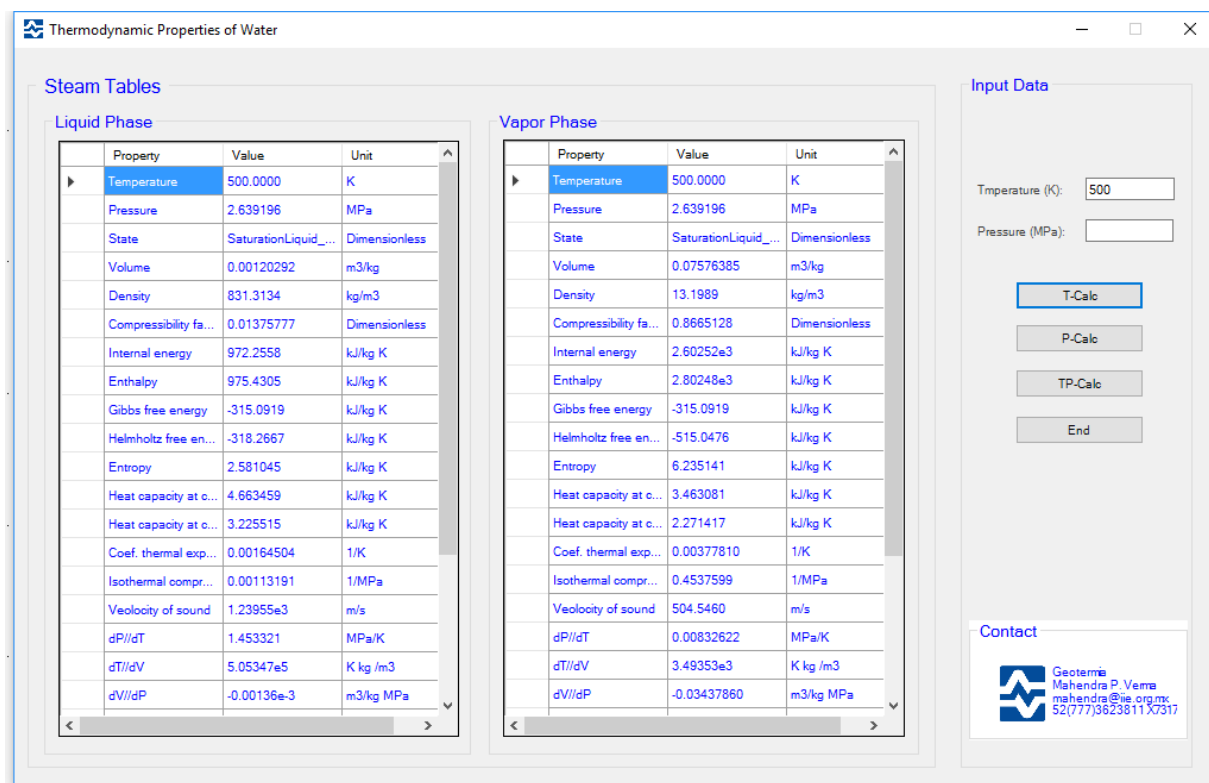


Figure 3: User graphic interface of demonstration program, *StmTblApp*. It shows the calculated values of water properties for T = 500 K.

The main form is to calculate the thermodynamic properties of water using the IAPWS-95 formulation (Figure 3). It displays the thermodynamic properties at the given temperature and/or pressure. The buttons T-Calc and P-Calc calculate the properties along the separation boundary (i.e. saturation curve and critical isochor) as a function of temperature and pressure, respectively. The button TP-Calc works for any point as a function of temperature and pressure. The user provides the values of temperature (K) and pressure (MPa) in the respective textboxes. The Figure 3 shows the calculated values for T=500 K, which is obtained on pressing the button, T-Calc.

3.2 Water Heating in a Vessel

This section presents an application for water-heating in vessel, developed in C# to illustrate the consuming of the steam tables web service.

Figure 4 shows the user interface of an experiment of water heating in a closed container of constant volume 1.0 m³. It clearly shows that the supercritical region is made of compressed liquid and superheated steam, and the critical isochor is the separation boundary between the liquid and vapor phase in the supercritical region.

3.3 Website for Thermodynamic Properties of Water

Under the project CEMIE-Geo, a website, <http://www.INEELGeoSteam.Net/WtrStmTbl> is developed using the web service, <http://www.INEELGeoSteam.NET/INEELSteamTables.aspx>. All the concepts on the steam tables developed so far are converted a web application. The application is developed in Angular, Version 4 for consuming of the steam tables web service (Angular, 2017). Angular is the most accepted framework for developing a web application, which is developed by Google. We will use the Angular-Cli for generating the project (Cli-Angular, 2017).

This website presents the basic concepts of renewable energy, thermodynamics, and the inconsistencies in the steam tables caused by incorrect measurement of specific heat capacity at constant pressure and volume.

4. CONCLUSIONS

The assembly *ThermoDataIIE.dll* written in VB.NET provides 23 thermodynamic properties of pure water. The assembly is based on the updated formulations: *IAPWS-95* for scientific use and *IAPWS-IF97* for industrial use. The outcomes of this study are summarized as follows

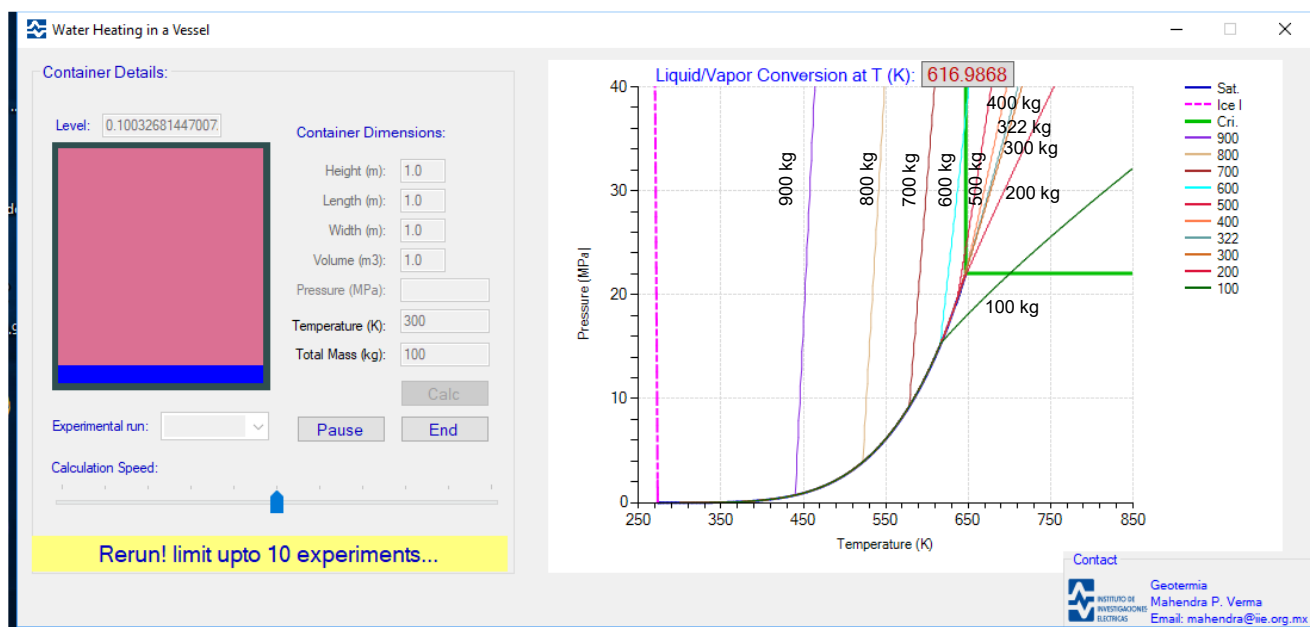


Figure 4: User graphic interface of water heating in a vessel. It shows the p-T diagram of heating water experiment for various amount of water in a vessel 1.0 m³.

1. The range of p-T surface for the *IAPWS-95* formulation is $T=190 - 2300$ K and $p= 3.23 \times 10^{-8} - 20617.8$ MPa; whereas for the *IAPWS-IF97* formulation it is $T=273.16 - 2273.15$ K and $p= 0.1 - 100.0$ MPa.
2. A web service, <http://www.INEELGeoSteam.NET/INEELSteamTables.aspx> is an interoperable (i.e., the web service built on a platform can consume in any other application on any platform).
3. The steam tables data have analytical uncertainties as $\Delta T = \pm 0.1$ K, $\Delta p = \pm 0.001$ MPa and $\pm 1\%$ in the calculated parameters.

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