RESEARCH ARTICLE

INEELSteamTables95: Excel Add-in for IAPWS-95 Scientific Formulation for Thermodynamic Properties of Pure Water and Steam and its Applications

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ABSTRACT

Steam tables of pure water are vital in many scientific and engineering applications, including the electric industry. Using the IAPWS-95 scientific formulation, an Excel add-in, INEELSteamTables95, was written in VBA to calculate 23 thermodynamic properties of pure water (i.e., steam tables). Its principal component is the class, Steam Tables. Using the Steam Tables class, various user-defined functions (UDF) were written in the Excel Personal Marcos Workbook to illustrate the add-in functionality in tabulating the steam tables and the Rankine power cycle calculations. A UDF, written in the Personal Marcos Workbook, can be used in any other workbook. Similarly, a user form was implemented to calculate the efficiency, production capacity, etc., of the Rankine power cycle, including the plots of s-T, v-p, and s-h diagrams based on the designed parameter values. The add-in and UDFs code (PersonalWorkbookFunctions.vb) are available on the first author's GitHub account, https://github.com/mpv55mx1Mex/INEELSteamTables95.git.

Keywords— Excel Add-in, IAPWS-95, Power Cycle, Steam Tables, Thermal Power Plant, VBA.

1 INTRODUCTION

MS Excel is one of the most popular platforms to perform scientific and engineering calculations: geothermal water and gas geochemistry [1], PVT calculation of MgO [2], acid-base titration curve [3], power cycle calculations [4], and others. In the above Excel examples, the thermodynamic properties of water play an essential role. Wagner and Pruβ [5] presented a comprehensive study on the evolution of thermodynamic formulations for pure water properties from the first formulation (IFC-68) to the most accepted IAPWS-95 formulation. The p-T computation schemes: IAPWS-95 for scientific use and IAPWS-IF97 for industrial use are widely accepted. Using the IAPWS-95 and IAPWS-IF97 formulations, many programmers wrote the dynamic link libraries (DLL) or assembly to get the reusability of steam tables of pure water in different programs [6], [7], [8], [9]. However, some compatibility issues exist in using a DLL developed with .NET technology (C# and Visual basic) in an Excel workbook based on COM technology [10]. Therefore, this work presents an add-in, INEELSteamTables95, for the steam tables of pure water, written VBA using the IAPWS-95 formulation to overcome the compatibility problem.

2 P-T PHASE DIAGRAM OF IAPWS-95 FORMULATION

Figure 1 shows the p-T surface of pure water, according to the IAPWS-95 formulations [6]. There are six separation boundaries marked with a roman number, I to VI, in a rectangle. The boundaries are *Sublimation, Saturation, Critical Isochor, IceI Melting, IceIII-VII Melting, Minimum Volume*, respectively. Along a separation boundary, there is only one independent variable, either T or p. Similarly, 16 states of water 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, 14-16 as phase regions). The states are denoted as *Triple Point, Critical Point, Minimum Volume Saturation Point, IceI-Liquid-Liquid1 Point, IceI-IceIII Point, Sublimation, Saturation Liquid-Vapor, Saturation Liquid1-Vapor, Critical Isochor, IceI-Liquid Curve, IceI-Liquid1 Curve, IceIII-IceVII Melting Curve, Minimum Volume Curve, Superheated Steam, Compressed Liquid, Compressed Liquid1*, respectively [6]. The minimum volume curve represents a separation boundary between "liquid" and "liquid I." The critical isochor represents the continuous liquid-vapor transformation.

Figure 2 shows tree diagrams to define in VBA for (a) class: Steam Tables, (b) enumerate: WtrProp Name, WtrSep-Boundary, and WtrState, and (c) structure: WtrProps and WtrProp Value. The class and structure encapsulate data and methods and serve as the blueprint for creating objects. A structure is a value type, while a class is a reference type. The functionality of a class and a structure may be extended without knowing its code [6].

3 INEELSTEAMTABLES95 EXCEL ADD-IN

An Excel add-in allows the creation of user-defined functions (UDF) and their use in different workbooks. First, create an Excel Workbook to store macros (i.e., with extension .xlsm).
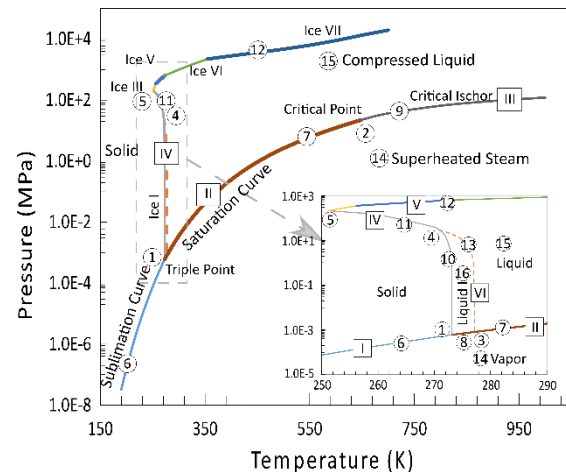

Fig. 1: p-T phase diagram of pure water, according to the IAPWS-95 formulation [6]. There are sixteen states marked with a number in a circle (1-5 as triple points, 6-13 as separation boundaries, 14-16 as phase regions), and six separation boundaries marked as a roman number I to VI in a rectangle. The inserted figure is an amplification to illustrate the triple points.

Using the IAPWS-95 formulation [5], a class Steam Tables is written in VBA for the properties and methods, as shown in Fig. 2a. Similarly, the enumerates and structures are defined in the module (Fig. 2b,c). The add-in INEELSteamTables95, and UDFs code here are available on the first author's GitHub account.

4 USING INEELSTEAMTABLES95 IN A WORKBOOK

The principal component of the add-in, INEELSteamTables95 is the SteamTables class (Fig. 2a). We will explain its use to write a function similar to the UDFs as given in Table 1. If you find difficulty in understanding the steps, search for help on the internet. The steps are the following

1. Install the add-in INEELSteamTables95 in your Excel: File – Options – Add-ins – Manage Excel-Add-ins – Go – Browse and select INEELSteamTables95.

2. Create a reference in the Excel Personal Workbook to the Add-in workbook (INEELSteamTable95.xlam): selecting the

Personal Workbook in the VBA editor – Tools – References… – Select Checkbox for the add-in workbook. Verma [6] explained the procedure for creating and writing code in the Excel Personal Workbook. The functions and macros written here can be used in any other workbook.

3. Figure 3 shows the code of SatPropsT function to explain the procedure to instantiate the Steam Tables class. Declare a global (or local) variable of the Steam Tables class. Excel does not permit the instantiation of a class outside the workbook; so, a function, NewSteam Tables was created within the add-in workbook for it [11]. The first line of the function, SatPropsT creates an instance of the class. Then assign the values of "SepBoundry" to "Saturation" and "Temperature" to the input value, Temp, and then execute the method, TUpdate. The function, SatPropsT provides the values of water properties. The function, AssignProps, converts the 23 properties of liquid and vapor in an array to display in a worksheet (Table 2). Now, if we change the value of temperature (273.16 to 647.096 K) in the worksheet, it will display water properties' values at the temperature. This way, we can exhibit the whole steam tables in the worksheet

4. Using these steps, a user can write any function based on the steam tables of pure water.

THERMODYNAMICS OF WATER-VAPOR POWER PLANT

Steam power plants for electricity generation utilize fuels like coal, oil, natural gas, geothermal heat, nuclear fuel, and biomass [12]. Thermodynamic process cycles are of two types:

power cycles, which produce a net power output, and refrigeration and heat pump cycles, which consume a net power input [13].

5.1 Rankine Power Cycle

The Rankine cycle, the thermodynamic vapor cycle, consists of a boiler, turbine, condenser, and pump (Figure 4). Fuel, burned in the boiler, heats the water to generate superheated steam. This steam runs the turbine, which powers the generator to produce electrical energy. After the steam leaves the turbine, it is cooled to its liquid state in the condenser by transferring heat to the cooling water system.

The pump pressurizes the liquid before going back to the boil. Fig. 4b shows a conceptual view of the four processes of an ideal Rankine cycle: 1-2 Isentropic compression in a pump, 2-3 constant pressure head addition in a boiler, 3-4 Isentropic expansion in a turbine, and 4-1 Constant pressure heat rejection in a condenser [13].

The theoretical concepts of energy analysis of four components of the Rankine power cycle are well described in the ebook [13]; so, these concepts are not repeated here.

Table 3 shows the calculated values of the working fluid's thermodynamic properties (i.e., water) for the design parameters (Condenser pressure = 0.008 MPa, Boiler pressure = 16.0 MPa, Steam temperature at the turbine inlet = 875 K, and Mass flow rate = 20 kg/s) at the points established in Fig. 4b. From the data of Table 3, the following parameters are calculated

The pump work input (isentropic compression)

$$W_{pump,in} = h_2 - h_1 = 14.18 \text{ kJ/kg}$$

Heat input at the boiler (constant pressure)

$$q_{in} = h_3 - h_2 = 3391.34 \text{ kJ/kg}$$

TABLE 1: Description of functions written using the class SteamTables of the add-in, INEELSteamTable95

Function	Input range	Description

TIce1, PIce1	T= 251.165 – 273.16 p= 6.11E-4 – 208.566	Temperature (K) or pressure (MPa) as the input parameter. Tice (PIce) calculates
TIce3, PIce3	T= 251.165 – 256.164 p= 208.566 – 350.1	temperature (T) as function pressure (p) and vice versa. Melt represents the curves
TIce5, PIce5	T= 256.164 – 273.31 p= 350.1 – 632.4	from Ice III to Ice VII.
TIce6, PIce6	T= 273.31 – 355 p= 632.4 – 2216	
TIce7, PIce7	T= 355 – 715 p= 2216 – 20618	
TMelt, PMelt	T= 251.165 – 715 p= 208.566 – 20618	
TSubl, PSubl	T= 190 – 273.16 p= 3.23 E-8 – 6.11E-4	Along sublimation curve
TMinVol, PMinVol	T= 270.96 – 277.15 p= 28.35 – 8.13E-4	Along the minimum volume curve [6]
TSat, PSat	T= 273.16 – 647.096 p= 6.11E-4 – 22.064	Along the liquid-vapor saturation curve from the triple point to the critical point
T_Ext, P_Ext	T= 647.096 – 2300 p= 22.064 – 432.84	Along the critical isochor [6]
SatPropsT, SatPropsP	T= 273.16 – 647.096 p= 6.11E-4 – 22.064	Calculate all the 23 properties of liquid and vapor along the saturation curve as T or p input parameter (enumerated properties in Fig. 2b)
NSatPropT, NSatPropP	Nprop = 1 – 23, Nphs = 1(liq), 2(vap) T= 273.16 – 647.096 p= 6.11E-4 – 22.064	Calculate one of the 23 properties of liquid or vapor along the saturation curve as T or p input parameter
PropsTP	T= 273.16 – 2300 p= 6.11E-4 – 20618	Calculate all the 23 properties of liquid and vapor at a given value of T and p
NPropTP	N = 1 – 23, Nphs = 1(liq), 2(vap) T= 273.16 – 2300 p= 6.11E-4 – 20618	Calculate one of the 23 of the properties of liquid or vapor at any given T and p

The turbine work output (isentropic expansion)

$$W_{turbine,out} = h_3 - h_4 = 1500.16 \text{ kJ/kg}$$

Heat rejection at the condenser (constant pressure)

$$q_{out} = h_4 - h_1 = 1905.36 \text{ kJ/kg}$$

The thermal efficiency of the Rankine cycle is

$$\eta_{net,out} = \frac{W_{net,out}}{q_{in}} = 1 - \frac{q_{out}}{q_{in}} = 43.82 \text{ \%}$$

where the net-work output from the cycle is

$$W_{net,out} = \left(W_{turbine,out} - W_{pump,in} \right) = 1486.00 \text{ kJ/kg}$$
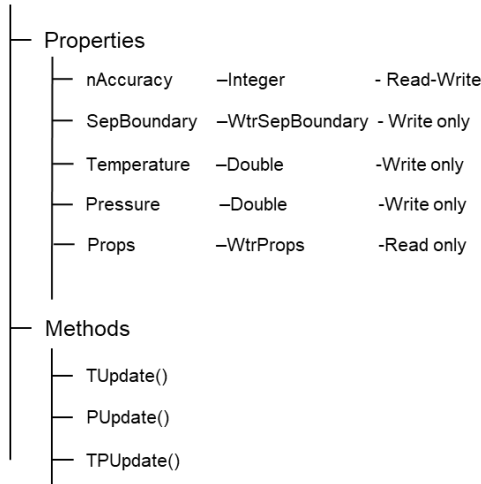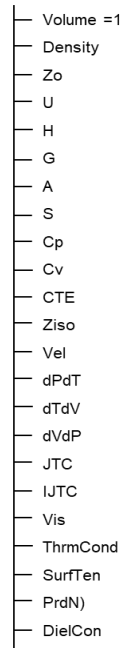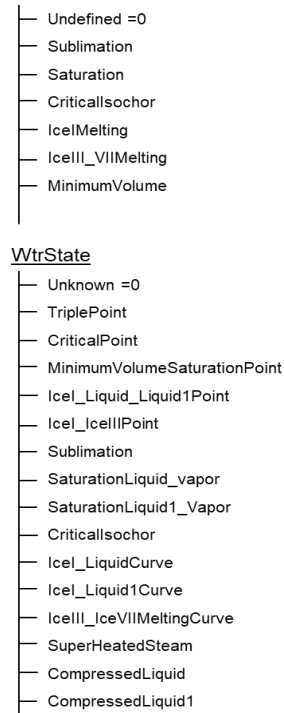
The power produced by the plant is

$$P = \dot{m} \times W_{net,out} = 29.72 \text{ MW}$$

The efficiencies of the pump and the turbine are considered to be 100%.

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SteamTables

```
│   Properties
│   │   nAccuracy      –Integer            - Read-Write
│   │   SepBoundary    –WtrSepBoundary    - Write only
│   │   Temperature    –Double            -Write only
│   │   Pressure       –Double            -Write only
│   │   Props          –WtrProps          -Read only
│   Methods
│   │   TUpdate()
│   │   PUpdate()
│   │   TPUpdate()
```

Fig. 2a

WtrPropName

```
│   Volume =1
│   Density
│   Zo
│   U
│   H
│   G
│   A
│   S
│   Cp
│   Cv
│   CTE
│   Ziso
│   Vel
│   dPdT
│   dTdV
│   dVdP
│   JTC
│   IJTC
│   Vis
│   ThrmCond
│   SurfTen
│   PrdN)
│   DielCon
```

WtrSepBoundary

```
│   Undefined =0
│   Sublimation
│   Saturation
│   CriticalIsochor
│   IceIMelting
│   IceIII_VIIMelting
│   MinimumVolume
```

WtrState

```
│   Unknown =0
│   TriplePoint
│   CriticalPoint
│   MinimumVolumeSaturationPoint
│   IceI_Liquid_Liquid1Point
│   IceI_IceIIIPoint
│   Sublimation
│   SaturationLiquid_vapor
│   SaturationLiquid1_Vapor
│   CriticalIsochor
│   IceI_LiquidCurve
│   IceI_Liquid1Curve
│   IceIII_IceVIIMeltingCurve
│   SuperHeatedSteam
│   CompressedLiquid
│   CompressedLiquid1
```

Fig. 2b

WtrProps

```
│   Temp       – Temperature (K)
│   Press      – Pressure (Pa)
│   State      – WtrState
│   Liquid     – WtrPropValue
│   Vapor      – WtrPropValue
```

WtrPropValue

```
│   Volume    – Volume  (m3/kg)
│   Density   – Density (kg/m3
│   Zo        – Compressibility Factor (dimensionless)
│   U         – Internal Energy (J/kg)
│   H         – Internal Energy (J/kg)
│   G         – Gibbs Free Energy (J/kg)
│   A         – Helmholtz Free Energy (J/kg)
│   S         – Entropy (J/(kg K)
│   Cp        – Heat Capacity at Constant Pressure (J/(kg K)
│   Cv        – Heat Capacity at Constant Volume  (J/((kg K))
│   CTE       – Coefficient of Thermal Expansion (1/K)
│   Ziso      – Isothermal Compressibility (1/Pa)
│   VelS      – Speed of Sound (m/s)
│   dPdT      – Partial Derivative of P with T at Constant V  (Pa/K)
│   dTdV      – Partial Derivative of T with V at Constant P  (m kg/m3)
│   dVdP      – Partial Derivative of V with P at Constant T  (m3/(kg Pa))
│   JTC       – Joule-Thomson Coefficient (K/Pa)
│   IJTC      – Isothermal Joule-Thomson Coefficient  (J/(kg Pa))
│   Vis       – Viscosity (Pa S)
│   ThrmCond  – Thermal Conductivity (W/(m K))
│   SurfTen   – Surface Tension (N/m)
│   PrdNum    – Prandtl Number (dimensionless)
│   DielCons  – Dielectric Constant (dimensionless)
```
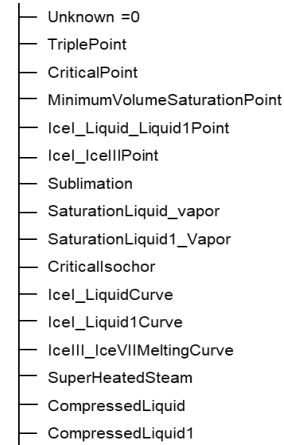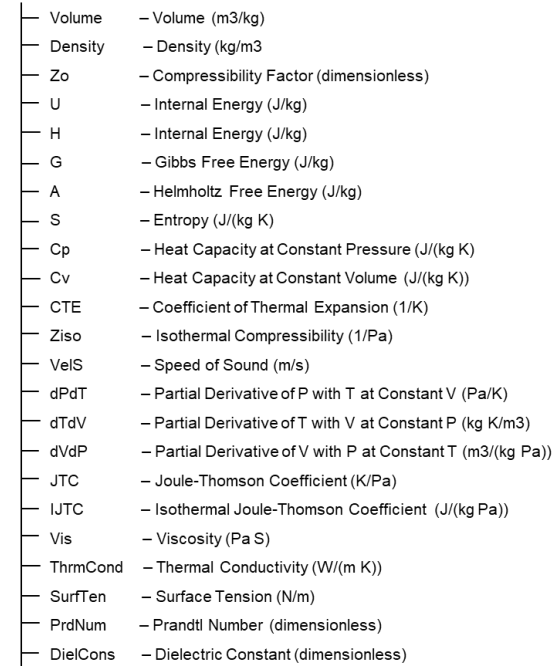
Fig. 2c

Fig. 2: Tree diagrams to illustrate the definitions of (a) class: SteamTables, (b) enumerate: WtrPropName, WtrSep-Boundary, and WtrState, and (c) structure: WtrProps and WtrPropValue, which were programmed in VBA.

```vba
Dim stmtbl As SteamTables            ← Create a variable
Public Function SatPropsT(Temp As Double) As Double()
    Set stmtbl = NewsteamTables      ← Instantiate

    Dim props As WtrProps

    stmtbl.SepBoundary = WtrSepBoundary.Saturation
    stmtbl.Temperature = Temp         ← Assign inputs
    stmtbl.TUpdate                    ← Execute method

    props = stmtbl.props              ← Water properties

    SatPropsT = AssignProps(props)    ← Convert Array
End Function
```

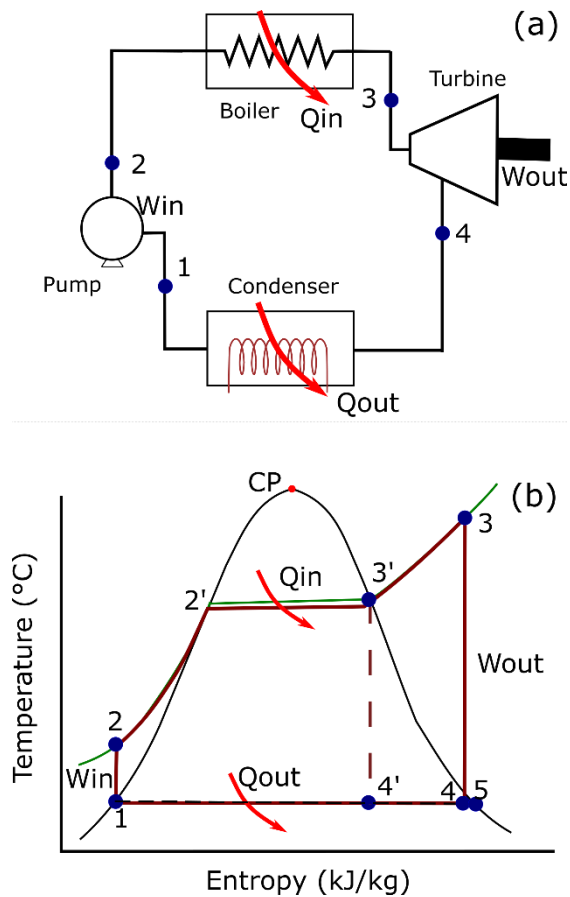Fig 3. Excel function code in VBA.

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	Temperature (K):	550	
	Pressure (MPa):	6.123403701	
S.No.	Property Name	Liquid	Vapor
1	Volume (m3/kg)	0.001323087	0.031725335
2	Density (kg/m3	755.8079163	31.52054997
3	Zo (dimensionless)	0.031885142	0.765328217
4	U (kJ/kg)	1212.379186	2588.634915
5	H (kJ/kg)	1220.472749	2782.901948
6	G (kJ/kg)	-451.211493	-451.014008
7	A (kJ/kg)	-459.3050559	-645.28104
8	S (kJ/(kg K))	3.039425894	5.879847192
9	Cp (kJ/(kg K))	5.233078585	4.942638947
10	Cv (kJ/(kg K))	3.091283806	2.721292438
11	CTE (1/K)	0.002497953	0.005491938
12	Ziso (1/MPa)	0.00212003	0.236921125
13	VelS (m/s)	1027.85645	493.1659118
14	dPdT (Pa/K)	1.178263152	0.023180447
15	dTdV (kg K/m3)	302570.881	5739.422427
16	dVdP (m3/(kg Pa))	-2.80499E-06	-0.0075164
17	JTC (K/Pa)	0.094527225	12.96941244
18	IJTC (kJ/(kg Pa))	-0.000494668	-0.06410312
19	Vis (Pa S)	94.74571436	18.56282759
20	ThrmCond (W/(m K))	0.585954151	0.059490898
21	SurfTen (N/m)	0.019729922	-1
22	PrdNum (dimensionless)	0.846161374	1.542241875
23	DielCons (dimensionless)	23.25203273	1.238181201

Fig. 4: Rankine power cycle: (a) schematic diagram, and (b) conceptual s-T diagram. Point 5 represents the vapor saturation point at the condenser pressure.

Figure 5 shows the s-T, v-p, and s-h diagrams for the above-designed parameters of an ideal Rankine power cycle. These calculations and graphs are programmed in an Excel workbook.

TABLE 2: Thermodynamic properties of water along the liquid-vapor saturation curve as a function of temperature

TABLE 3: Thermodynamic properties of water at the Ideal Rankine cycle points (Fig. 4b)

Point	P (MPa)	T (K)	V (m³/kg)	H (kJ/kg)	S (kJ/kg-K)	Vapor fraction
1-	0.008	314.646	0.001	173.786	0.592	0.000
2-	16.000	314.677	0.001	187.969	0.592	0.000
2'-	16.000	620.450	0.002	1649.260	3.745	0.000
3'-	16.000	620.450	0.009	2579.957	5.245	1.000
3-	16.000	875.000	0.023	3579.310	6.648	1.000
4'-	0.008	314.646	11.029	1637.777	5.245	0.609
4-	0.008	314.646	14.354	2079.149	6.648	0.793
5-	0.008	314.646	18.098	2576.181	8.227	1.000

Similarly, a user form (Figure 6) is designed to handle the calculations in a friendly manner. Changing the design parameter values and pressing the button, Calculate, it automatically performs all the calculations and shows the frame's results in Fig. 6. It also replots the s-T, v-p, and s-h diagrams, displayed in the Picturebox on selecting the respective name from the Combobox, Phase diagram.

The Rankine power cycle is generally shown in the literature by schematic phase diagrams. The actual phase diagrams developed based on water's

thermodynamic properties provide insight into designing the power plant.

In the boiler, the liquid and vapor water coexist up to T=620.45 K and P=16.00 MPa. On further heating (T=875 K) the vapor at the constant pressure, there should not be any liquid phase, with a vapor volume increase by a factor of 2.5 times. Similarly, the turbine's exhausted steam converts into the liquid-vapor phase with vapor fraction 0.793 and volume expansion by 616 times. These calculations help to design the power plant. Additionally, the effect of various parameters on the plant design can be studied by changing that parameter's value in the Excel worksheet, as it performs all the calculations.

6   S-H PHASE DIAGRAM OF PURE WATER

Figure 7 shows the s-h phase diagram of pure water, developed using the IAPWS-95 scientific formation in Ex-cel. The software is written as temperature and pressure as input parameters. In other words, the T-p phase diagram (Fig. 1) was mapped in the s-h phase diagram (Fig. 6). Fig. 6a shows the isotherm. It can be observed that there are multiple-values in the compressed liquid region.

There are two entropy values (4.20 and 5.03 kJ/kg-K) at the enthalpy 2850 kJ/kg for the isotherm T=990K (see points 2 and 3). Similarly, the isotherm T=700K has the same enthalpy, 2850 kJ/kg for the vapor and liquid phases (Points 1 and 4), but different entropy values, 2.87 and 5.60 kJ/kg-K.
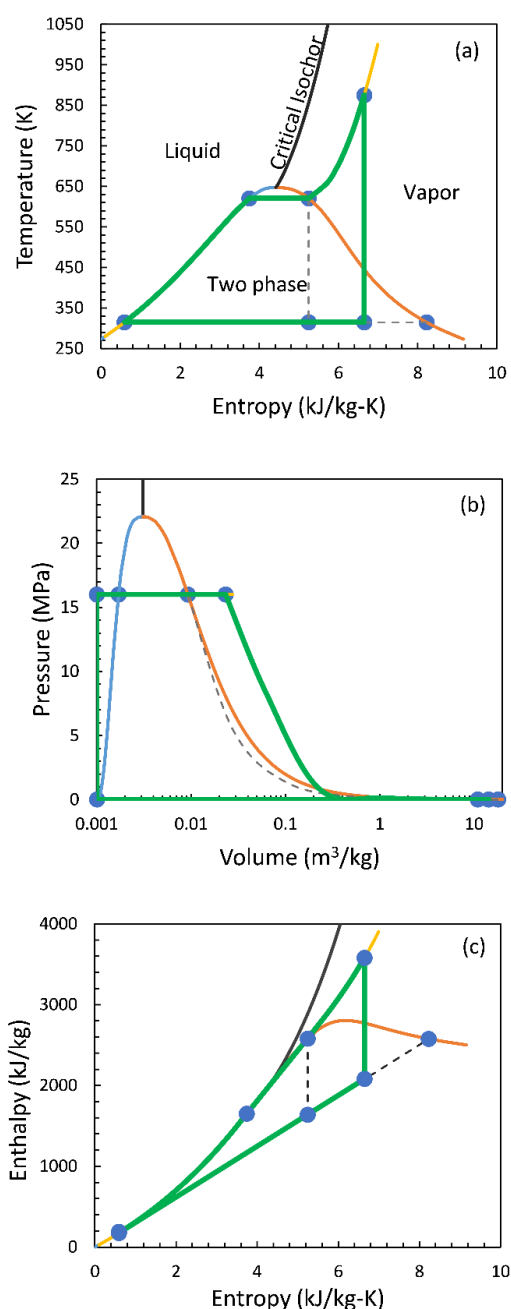

Fig. 5: Rankine power cycle representation in the phase diagrams: (a) s-T diagram, (b) v-p diagram, and (c) s-h diagram. The dot-points nomenclature is in Figure 4b.
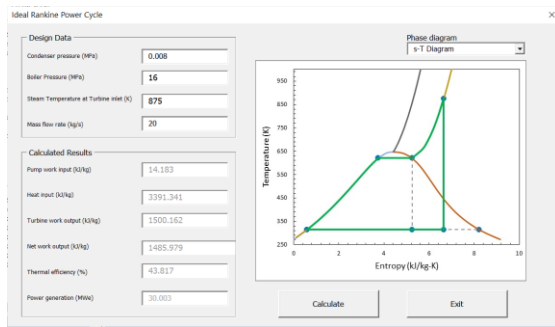
Fig. 6: User form for the data analysis and visualization of Rankine power plant's thermodynamic diagrams written in VBA.

In Fig. 6b, the isobars in the liquid region are close to the saturation curve. It means that the s-h relation in the liquid region is independent of pressure.

7   CONCLUDING REMARKS

The add-in, INEELSteamTables95 written in VBA, provides 23 thermodynamic properties of pure water. The add-in is implemented based on the most accepted formulations: IAPWS-95 for scientific use. The outcomes of this study are summarized as follows

1.   The range of p-T surface for the IAPWS-95 formulation is T=190 – 2300 K and p= 3.23×10^{-8} – 20617.8 MPa.

2.   The user-defined functions were written in the Personal Marcos Workbook using the INEELSteamTables add-in, which permits the development of different surfaces for the steam tables of pure water (e.g., s-h surface presented here) in a friendly manner.

3.   The multiple values on the isotherms and the pressure independence of the s-h relation in the compressed liquid region (Fig. 6) are severe issues for the thermodynamic inconsistency in the steam tables of pure water.
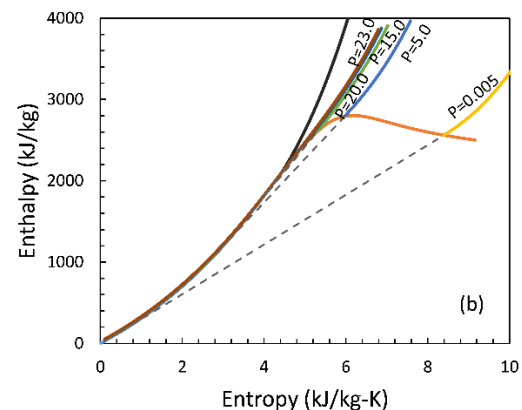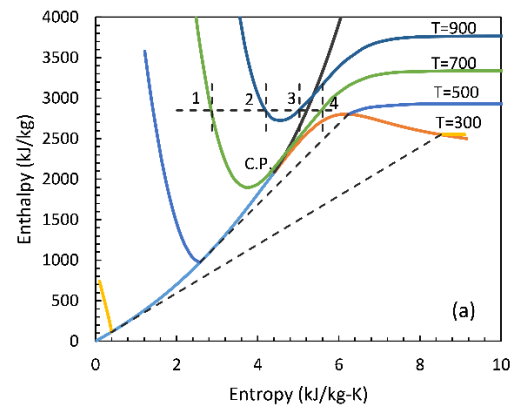

Fig. 7: s-h phase diagram of pure water, based on the IAPWS-95 scientific formulation

4.   The Rankine power cycle application presented here is beneficial for the engineers working on the electric power plants' design and operation.

5.   The add-in, INEELSteamTables95, can be used in any calculations needed for water's thermodynamic properties.

References

[1]   T. Powell and W. Cumming, "Spreadsheets for geothermal water and gas geochemistry," Proceedings, Thirty-Fifth Workshop on Geothermal Reservoir

Engineering Stanford University, Stanford, California, USA, 2010.

[2] T.S. Sokolova, P.I. Dorogokupets, A.M. Dymshits, B.S. Danilov and K.D. Litasov, "Microsoft Excel spreadsheets for calculation of P-V-T relations and thermodynamic properties for equations of state of MgO, diamond and nine metals as pressure markers in high-pressure and high-temperature experiments," Comput. Geosci., vol. 94, 2016, pp. 162-169.

[3] I.G. Rolf-Gutz, "pH calculation + virtual titration + acid-base titration curve data analysis + distribution diagram generation + pKa database = CurTiPot," http://www.iq.usp.br/gutz/Curtipot_.html

[4] B. Dan-Asabe and D.S. Yawas, "Design, simulation and optimization of a three-stage gas turbine cycle using Microsoft Excel," Nigerian Journal of Engineering, vol. 18(1), 2011, pp. 145-152.

[5] W. Wagner and A. Pruβ, "The IAPWS formulation 1995 for the thermodynamic properties of ordinary water substance for general and scientific use," J. Phys. Chem. Ref. Data, vol. 31(1), 2002, pp. 387-535.

[6] M.P. Verma, "Steam tables for pure water as an ActiveX component in Visual Basic 6.0," Compu. Geosci., vol. 29(9), 2003, pp. 1155-1163.

[7] M.P. Verma, "Steam tables: an approach of multivariable sets," Compu. Geosci., vol. 35, 2009, pp.2145-2150.

[8] X.D. Wang, B. An, Y.Y. Duan, Z.X. Wang and D.J. Lee, "Efficient and accurate computation scheme of p-T thermodynamic properties of water and steam," J. Taiwan Inst. Chem. Eng. Vol. 43, 2012, pp. 845-851.

[9] M.P. Verma, "p-T computation schemes for thermodynamic properties of pure water: a comparative evaluation of IAPWS95 and IAPWS-IF97 formulations," In: Janardhana,

R.N. (ed.) Geostatistical and geospatial approaches for the characterization of natural resources in the environment: Challenges, processes and strategies. Springer, Capital Publishing Company: New Delhi, 2016, pp.101-104.

[10] R. Newman, "A beginner's guide to calling a .NET framework library from Excel," https://richnewman.wordpress.com/2007/04/15/a-beginners-guide-to-calling-a-net-library-from-excel/

[11] https://docs.microsoft.com/en-us/previous-versions/office/troubleshoot/office-developer/set-up-vb-project-using-class

[12] M.A. Khattak, M.A. Ashraff, M. Ikmal, A. Syafig, and M. Hazritz, "Common types of fuels in steam power plant: a review," Journal of Advanced Research in Fluid Mechanics and Thermal Sciences, vol. 23, 2016, pp. 1-24.

[13] http://www.ecourses.ou.edu/cgi-bin/ebook.cgi?doc=&topic=th&chap_sec=10.0.

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