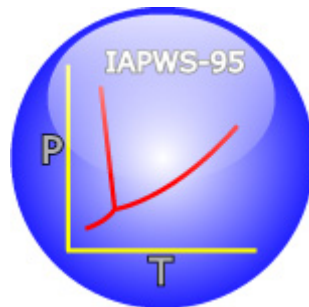


PhaseCalc for Steam Version 1.0



Engineering software prepared by

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Table of Contents

Table of Contents	2
Introduction	3
Program Capabilities	4
Program Input	7
Flash Conditions	7
Units	8
Program Output	10
Main Screen	10
Printed Reports	10
Display Precision	11
Fluid Properties on the Saturation Curve	11
Technical Support	12
References	13
Appendices	14
Appendix A: Examples	14
1. Saturated Mixture at 450 K with Quality of 75%	14
2. Superheated Steam at 30 MPa with Enthalpy of 4000 kJ/kg	15
3. IAPWS-95 Validation	16
Appendix B: Software Installation and Setup	17

Introduction

PhaseCalc for Steam (PhaseCalc) is an implementation of the internationally recognized fundamental equation for the fluid properties and phase behavior of water. The International Association for the Properties of Water and Steam (IAPWS) web site at <http://www.iapws.org> contains details of the 1995 Release of the Scientific Formulation¹ (IAPWS-95) on which *PhaseCalc* is based. This model was chosen over the 1997 Industrial Formulation² (IF97) because of its thermodynamic consistency over the entire range of pressure and temperature, and because of its superior accuracy. More information about the IAPWS-95 implementation developed by Tomcej Engineering Inc. (Tomcej) is available on the Tomcej web site at <http://www.tomcej.com>.

PhaseCalc can be used to predict the properties of water and steam over a wide range of pressures and temperatures of industrial interest. It can be used to analyze the performance of process equipment such as compressors, valves or pipeline systems, where water or steam is involved. *PhaseCalc* also includes an implementation of the IAPWS formulation for dynamic viscosity³ and thermal conductivity⁴ to assist in these process calculations.

Program Capabilities

PhaseCalc runs essentially like a spreadsheet. By specifying any two independent properties and/or a condition from a given set of options, the program solves for the remaining properties. At present, the program will calculate the following properties:

Table 1. Primary Properties Calculated by PhaseCalc

Property	Symbol
Pressure	P
Temperature	T
Density	ρ
Volume	v
Internal Energy	U
Enthalpy	H
Entropy	S
Isochoric Heat Capacity	C_v
Isobaric Heat Capacity	C_p
Sonic Velocity	w
Joule Thomson Coefficient	μ_{JT}
Dynamic Viscosity	μ
Thermal Conductivity	k

Other secondary property values are also included in the program output. These include:

Table 2. Secondary Properties Calculated by PhaseCalc

Property	Symbol
Heat Capacity Ratio	C_p/C_v
Fugacity	f
Compressibility Factor	$Z=Pv/RT$
Mass or Mole % Vapor (Quality)	x
Volume % Vapor	y

At present, the following set of specifications may be used to initiate a flash calculation. These specifications apply to any region: the subcooled liquid region, the superheated vapor region, or the saturated vapor-liquid curve.

Table 3. Available Calculations

Specification	<i>PhaseCalc</i> Nomenclature
T and x on the Saturation Curve	Saturation P at T
P and x on the Saturation Curve	Saturation T at P
P and T	Flash at P and T
P and H	Flash at P and H
P and S	Flash at P and S
P and ρ	Flash at P and Density
T and H	Flash at T and H
T and S	Flash at T and S
T and ρ	Flash at T and Density
Critical Point	Critical Point

Figure 1 shows the main program screen that is displayed when the first specification option (Saturation P at T) is selected using a temperature of 300 K and 50 mass % vapor on the saturation curve.

Figure 1. Main Program Screen

The screenshot displays the 'PhaseCalc for Steam' application window. The title bar includes the application name and standard window controls. The menu bar contains 'File', 'View', 'Calculation', 'Tools', and 'Help'. The main content area is titled 'Fluid Properties at a Single Condition'. On the left, there is a 'Select Calculation:' section with several buttons: 'Saturation P at T' (selected), 'Saturation T at P', 'Flash at P and T', 'Flash at P and H', 'Flash at P and S', 'Flash at P and Density', 'Flash at T and H', 'Flash at T and S', 'Flash at T and Density', and 'Critical Point'. The main area contains a table of properties for Liquid, Vapor, and Feed states, along with their units. A 'Note:' field is located at the bottom left.

Property	Liquid	Vapor	Feed	Units
Pressure			3.53681	kPa
Temperature			300	K
Density	996.513	0.0255897	0.051178	kg/m ³
Volume	0.0010035	39.0783	19.5396	m ³ /kg
Molar Mass	18.0153	18.0153	18.0153	kg/kmol
Internal Energy	112.561	2411.64	1262.1	kJ/kg
Enthalpy	112.565	2549.85	1331.21	kJ/kg
Entropy	0.393089	8.51739	4.45524	kJ/kg·K
Heat Capacity, Cv	4.1305	1.44224	2.78637	kJ/kg·K
Heat Capacity, Cp	4.18091	1.91408	3.0475	kJ/kg·K
Cp/Cv	1.01221	1.32716	1.09372	-
Fugacity	3.53072	3.53072		kPa
Z=Pv/RT	2.56341E-05	0.998244	0.499135	-
Mole %	50	50	100	%
Mass %	50	50	100	%
Volume %	0.00256786	99.9974	100	%
Sonic Velocity	1501.36	427.89		m/s
Joule Thomson	-0.220239	264.352		K/kPa
Dynamic Viscosity	853.843	9.91953		μPa·s
Thermal Conductivity	610.278	18.6732		mW/m·K

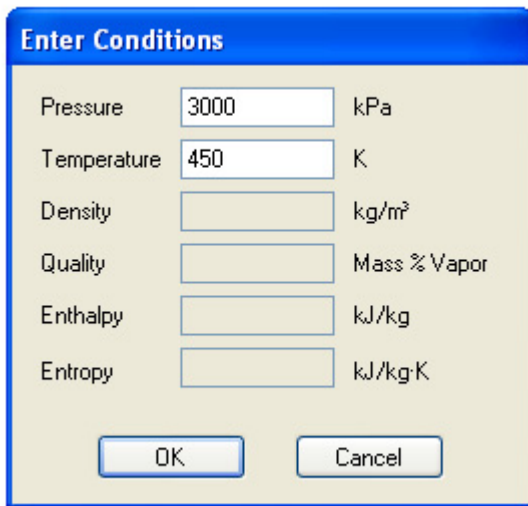
www.tomcej.com Note:

Program Input

Flash Conditions

Specifications for the conditions are entered in the Flash Conditions dialog shown in Figure 2.

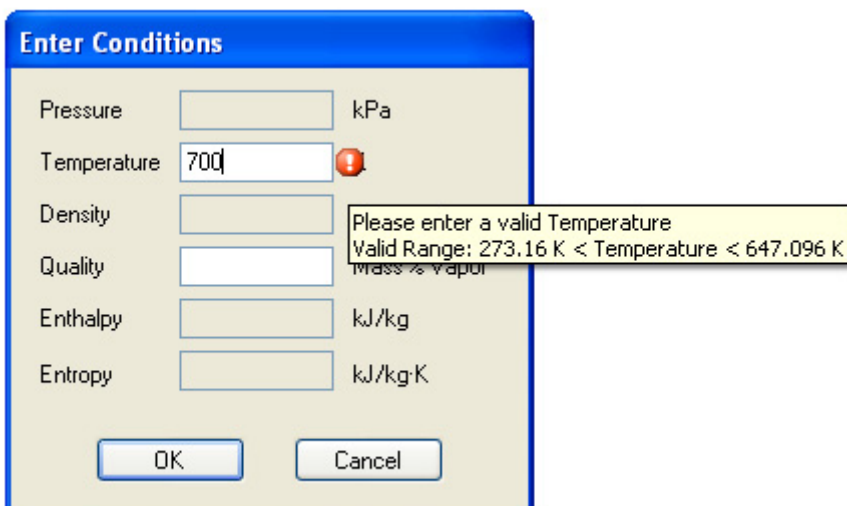
Figure 2. Flash Conditions Dialog Box



The dialog box titled "Enter Conditions" has a blue header. It contains six input fields with labels and units to their right: Pressure (3000 kPa), Temperature (450 K), Density (kg/m³), Quality (Mass % Vapor), Enthalpy (kJ/kg), and Entropy (kJ/kg·K). At the bottom are "OK" and "Cancel" buttons.

The Flash Conditions dialog is presented when one of the calculation buttons on the main screen is pressed, or a menu item on the Calculation menu is selected. Depending on which calculation option is selected, the program will request only the required information. The input values are validated prior to performing the calculation to ensure they fall within the acceptable range. A notification message is displayed if the entered values are invalid. An example of this is shown in Figure 3.

Figure 3. Validation of Input Data



The dialog box titled "Enter Conditions" shows the Temperature field with the value "700" and a red error icon. A tooltip message is displayed over the error icon: "Please enter a valid Temperature
Valid Range: 273.16 K < Temperature < 647.096 K". The other fields and buttons are the same as in Figure 2.

In this example, an invalid temperature has been entered in a saturated steam calculation. If the entered values pass the data validation process, the program proceeds with the selected calculation.

Units

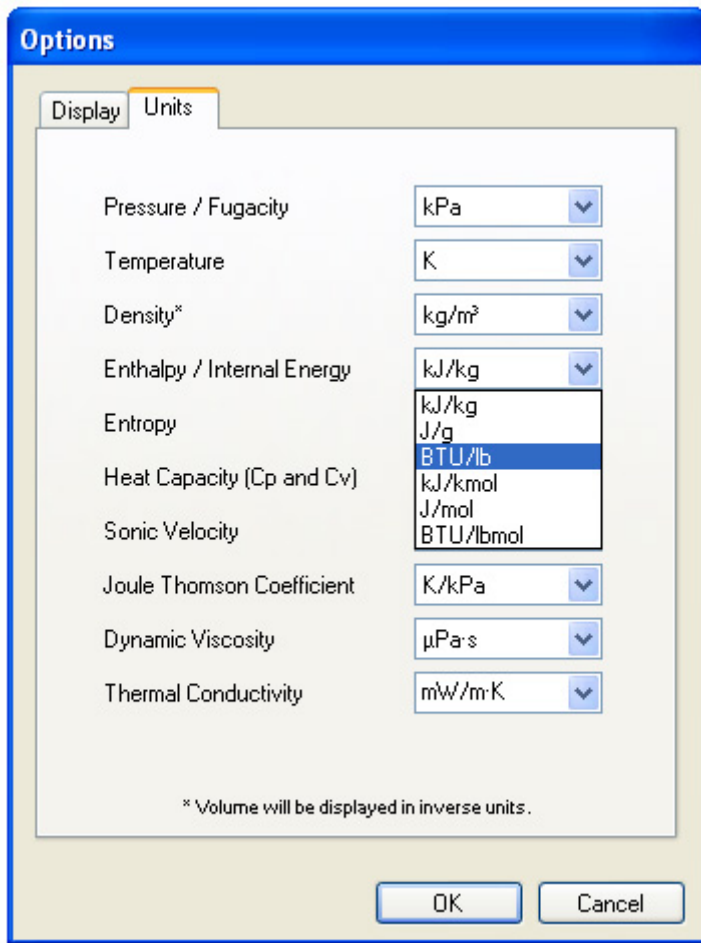
PhaseCalc uses SI units for internal calculations as this is the basis of the IAPWS-95 formulation. Input and output may be displayed in other unit systems for convenience. At present, the following units are available for use:

Table 4. Available Unit Systems

Property	Units
Pressure, Fugacity	kPa, psi, atm, MPa, bar, mm Hg
Temperature	K, °R, °C, °F
Density	kg/m ³ , g/cm ³ , lb/ft ³ , kmol/m ³ , mol/cm ³ , lbmol/ft ³
Volume	m ³ /kg, cm ³ /g, ft ³ /lb, m ³ /kmol, cm ³ /mol, ft ³ /lbmol
Internal Energy, Enthalpy	kJ/kg, J/g, BTU/lb, kJ/kmol, J/mol, BTU/lbmol
Entropy, Heat Capacity	kJ/kg·K, J/g·K, BTU/lb·°R, kJ/kmol·K, J/mol·K, BTU/lbmol·°R
Sonic Velocity	m/s, ft/s
Joule Thomson Coefficient	K/kPa, K/MPa, °F/psi, K/bar
Dynamic Viscosity	Pa·s, mPa·s, μPa·s, cP, lb/ft·h
Thermal Conductivity	W/m·K, mW/m·K, BTU/s·ft·°R, BTU/h·ft·°R

The preferred units may be selected in two ways. The Tools menu contains an Options menu item that presents the Options dialog box shown in Figure 4.

Figure 4. Selection of Default Units



By selecting the Units tab in the dialog box, the preferred units system may be entered by selecting values from the appropriate combo boxes. For example, Figure 4 shows the selection of BTU/lb as the preferred unit system for enthalpy. When the Options dialog is closed, the selected units become the new default system. These units will be displayed when requesting program input, when displaying or printing results, and the next time *PhaseCalc* is started.

As an alternative, the units for a particular property may be changed on the main screen in the Units column. The Units column includes a number of combo boxes that contain the available units for that particular property. By selecting a different set of units, the displayed property values for liquid, vapor and overall feed will be converted to the new units system. As with the options dialog box, units selected on the main screen may be saved as the new default system. When *PhaseCalc* is closed, the program will request confirmation to save the new units as the default system.

Program Output

Main Screen

Calculation results are displayed in the grid on the main screen. An example of the main screen display is shown in Figure 1.

Printed Reports

Results may also be printed or previewed by selecting the Print or Print Preview items on the File menu. An example of a printed report is given in Figure 5.

Figure 5. Example Printed Report

PhaseCalc for Steam				
Licensed to: Tomcej Engineering Inc.				Version 1.0.0251.0
Note:	Unit A - Pump P-102, Test Run 534			
VLE Model:	IAPWS-95			
Properties				
Pressure	932.203			kPa
Temperature	450			K
Density	890.341	4.812	12.8615	kg/m ³
Volume	0.00112316	0.207814	0.0777514	m ³ /kg
Molar Mass	18.0153	18.0153	18.0153	kg/kmol
Internal Energy	748.114	2580.69	1427.52	kJ/kg
Enthalpy	749.161	2774.41	1500	kJ/kg
Entropy	2.10866	6.60921	3.77719	kJ/kg·K
Heat Capacity, Cv	3.40768	1.90737	2.85146	kJ/kg·K
Heat Capacity, Cp	4.39273	2.67423	3.75561	kJ/kg·K
Cp/Cv	1.28907	1.40205	1.31709	
Fugacity	875.701	875.701		kPa
Z=Pv/RT	0.00504142	0.932789	0.348994	
Mole %	62.9261	37.0739	100	
Mass %	62.9261	37.0739	100	
Volume %	0.909005	99.091	100	
Sonic Velocity	1400.37	500.412		m/s
Joule Thomson	-0.117668	30.3071		K/kPa
Dynamic Viscosity	152.978	14.9171		μPa·s
Thermal Conductivity	674.586	35.9038		mW/m·K

The main screen includes a text box labeled “Note:”. Any project reference or title that is entered in this box will be included in the printed report.

Display Precision

For purposes of reproducing the results in the IAPWS guidelines, the number of digits displayed on the main screen and in the printed report may be adjusted on the Digits tab of the Options dialog box. The Options dialog is displayed by selecting the Options item on the Tools menu. The default display precision is six digits or less.

Fluid Properties on the Saturation Curve

For convenience, when calculations are performed on the saturated vapor-liquid curve, the numerical difference between the saturated vapor and saturated liquid values of either internal energy, enthalpy or entropy may be displayed by right-clicking the appropriate row on the main screen. Figure 6 shows the display when the entropy row is right-clicked.

Figure 6. Special Output Displayed on Right Click

The screenshot shows the PhaseCalc for Steam application window. The main window displays a table of fluid properties for a single condition. The 'Entropy' row is highlighted, and a small dialog box is overlaid on it, showing the calculated entropy difference between vapor and liquid phases.

Property	Liquid	Vapor	Feed	Units
Pressure			5000	kPa
Temperature			537.091	K
Density	777.369	25.3512	33.4381	kg/m ³
Volume	0.00128639	0.0394459	0.029906	m ³ /kg
Molar Mass	18.0153	18.0153	18.0153	kg/kmol
Internal Energy	1148.21	2596.98	2234.78	kJ/kg
Enthalpy	1154.64	2794.21	2384.31	kJ/kg
Entropy	2.92099	5.97367	5.2105	kJ/kg·K
Heat Capacity, Cv	3.12039		426	kJ/kg·K
Heat Capacity, Cp	5.03684		772	kJ/kg·K
Cp/Cv	1.61417		402	-
Fugacity	4195.02			kPa
Z=Pv/RT	0.025948		3243	-
Mole %	25	75	100	%
Mass %	25	75	100	%
Volume %	1.07536	98.9246	100	%
Sonic Velocity	1087.81	498.043		m/s
Joule Thomson	0.047232	14.3617		K/kPa
Dynamic Viscosity	100.006	18.0321		μPa·s
Thermal Conductivity	604.155	55.2031		mW/m·K

Special Output Dialog:

```

PhaseCalc for Steam
Entropy
Vapor - Liquid = 3.05268
OK
  
```

Technical Support

Owners of a registered copy of *PhaseCalc for Steam* have access to unlimited technical support. Please send support requests by e-mail to support@tomcej.com. Include a description of the problem and your contact information. Tomcej will make every effort to respond to your request in a timely manner. The “Technical Support Issue” menu item on the Help menu may be used to initiate a technical support request.

Although e-mail is the preferred method of technical support, requests may also be sent by telefax to our head office at 1.780.483.0248.

A current list of known technical issues and the status of their resolution is posted on the Tomcej Engineering web site at <http://www.tomcej.com/support/phasecalc/steam/knownissues.htm>. Please check this list to determine whether your problem is a known issue, prior to submitting a support request.

References

1. “Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use”, The International Association for the Properties of Water and Steam, Presented at Fredericia, Denmark, September 1996. (<http://www.iapws.org/relguide/IAPWS95.pdf>).
2. “Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam”, The International Association for the Properties of Water and Steam, Presented at Erlangen, Germany, September 1997. (<http://www.iapws.org/relguide/IF97.pdf>)
3. “Revised Release on the IAPWS Formulation 1985 for the Viscosity of Ordinary Water Substance”, The International Association for the Properties of Water and Steam”, Presented at Vejle, Denmark, August 2003. (<http://www.iapws.org/relguide/visc.pdf>)
4. “Revised Release on the IAPWS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substance”, The International Association for the Properties of Water and Steam”, Presented at London, England, September 1998. (<http://www.iapws.org/relguide/thcond.pdf>)

Appendices

Appendix A: Examples

It is assumed in these examples that the default units are kPa, K and kJ/kg for P, T and H respectively, and that the default precision is 9 digits.

1. Saturated Mixture at 450 K with Quality of 75%

- Click “Saturation P at T” or select the “Saturation p at T” item on the Calculation menu
- Enter “450” in the temperature box and “75” in the mass 5 vapor box
- Click OK or press Enter on the keyboard
- The following results are displayed on the main screen

Figure 7. Screen Display for Example A1

The screenshot shows the PhaseCalc for Steam software interface. The window title is "PhaseCalc for Steam". The menu bar includes "File", "View", "Calculation", "Tools", and "Help". The main window is titled "Fluid Properties at a Single Condition". On the left, there is a "Select Calculation:" section with several buttons: "Saturation P at T", "Saturation T at P", "Flash at P and T", "Flash at P and H", "Flash at P and S", "Flash at P and Density", "Flash at T and H", "Flash at T and S", "Flash at T and Density", and "Critical Point". The "Saturation P at T" button is selected. The main area displays a table of fluid properties for Liquid, Vapor, and Feed states. The units are specified in the "Units" column. At the bottom left, there is a website link "www.tomcej.com" and a "Note:" field.

Property	Liquid	Vapor	Feed	Units
Pressure			932.203564	kPa
Temperature			450	K
Density	890.34125	4.8120036	6.40446678	kg/m ³
Volume	0.00112316485	0.207813643	0.156141024	m ³ /kg
Molar Mass	18.015268	18.015268	18.015268	kg/kmol
Internal Energy	748.114566	2580.68616	2122.54326	kJ/kg
Enthalpy	749.161585	2774.41078	2268.09848	kJ/kg
Entropy	2.10865845	6.60921221	5.48407377	kJ/kg·K
Heat Capacity, Cv	3.4076775	1.90737264	2.28244885	kJ/kg·K
Heat Capacity, Cp	4.39272624	2.67422614	3.10385117	kJ/kg·K
Cp/Cv	1.28906748	1.40204703	1.35987764	-
Fugacity	875.701755	875.701755		kPa
Z=Pv/RT	0.00504142208	0.932789418	0.700852419	-
Mole %	25	75	100	%
Mass %	25	75	100	%
Volume %	0.1798318	99.8201682	100	%
Sonic Velocity	1400.37167	500.412284		m/s
Joule Thomson	-0.117668386	30.307077		K/kPa
Dynamic Viscosity	152.977937	14.9170827		μPa·s
Thermal Conductivity	674.585553	35.9038225		mW/m·K

2. Superheated Steam at 30 MPa with Enthalpy of 4000 kJ/kg

- Click “Flash at P and H” or select the “Flash at P and H” item on the Calculation menu
- Enter “30000” in the pressure box and “4000” in the enthalpy box
- Click OK or press Enter on the keyboard
- The following results are displayed on the main screen

Figure 8. Screen Display for Example A2

The screenshot shows the PhaseCalc for Steam software interface. The window title is "PhaseCalc© for Steam". The menu bar includes "File", "Calculation", "Tools", and "Help". The main area is titled "Fluid Properties at a Single Condition". On the left, there is a "Select Calculation:" section with several buttons: "Saturation P at T", "Saturation T at P", "Flash at P and T", "Flash at P and H" (highlighted), "Flash at P and S", "Flash at P and Density", "Flash at T and H", "Flash at T and S", "Flash at T and Density", and "Critical Point". The main table displays the following properties:

Property	Liquid	Vapor	Feed	Units
Pressure			30000	kPa
Temperature			1065.77234	K
Density			64.5698137	kg/m ³
Volume			0.015487113	m ³ /kg
Molar Mass			18.015268	kg/kmol
Internal Energy			3535.38661	kJ/kg
Enthalpy			4000	kJ/kg
Entropy			6.81132277	kJ/kg-K
Heat Capacity, Cv			2.00416597	kJ/kg-K
Heat Capacity, Cp			2.71639139	kJ/kg-K
Cp/Cv			1.35537247	-
Fugacity			28361.3567	kPa
Z=Pv/RT			0.944579651	-
Mole %			100	%
Mass %			100	%
Volume %			100	%
Sonic Velocity			772.426374	m/s
Joule Thomson			1.78535973	K/kPa
Dynamic Viscosity			42.2114434	μPa·s
Thermal Conductivity			130.53457	mW/m·K

At the bottom left, there is a link to www.tomcej.com. At the bottom right, there is a "Note:" field.

3. IAPWS-95 Validation

The following properties have been extracted from the IAPWS-95 guideline and may be used to confirm that the PhaseCalc program reproduces the published values

Table A-3.1 Thermodynamic Properties in the Single-Phase Region

T/K	ρ /(kg/m ³)	P/kPa	C_v /(kJ/kg·K)	w/(m/s)	S(kJ/kg·K)
300	996.5560	99.242	4.13018111	1501.51914	0.393062642
	1005.308	20002.2514	4.06798347	1534.92501	0.387405401
	1188.202	700004.704	3.46135580	2443.57992	0.132609616
500	0.4350000	99.9679423	1.50817541	548.314253	7.94488271
	4.532000	999.938125	1.66991025	535.739001	6.82502725
	838.0250	10000.3858	3.22106219	1271.28441	2.56690918
	1084.564	700000.405	3.07437693	2412.00877	2.03237509
647	358.0000	22038.4756	6.18315728	252.145078	4.32092307
900	0.2410000	100.062559	1.75890657	724.027147	9.16653194
	52.61500	20000.0690	1.93510526	698.445674	6.59070225
	870.7690	700000.006	2.66422350	2019.33608	4.17223802

Table A-3.2 Thermodynamic properties in the Two-Phase Region

T/K	P/kPa	ρ_L /(kg/m ³)	ρ_V /(kg/m ³)	H_L /(kJ/kg)	H_V /(kJ/kg)	S_L /(kJ/kg·K)	S_V /(kJ/kg·K)
275	0.698451167	999.887406	0.00550664919	7.75972200	2504.28995	0.0283094669	9.10660120
450	932.203564	890.341250	4.81200360	749.161585	2774.41078	2.10865845	6.60921221
625	16908.2693	567.090385	118.290280	1686.26976	2550.71625	3.80194683	5.18506121

Appendix B: Software Installation and Setup

PhaseCalc is based on the [.NET Framework 2.0](#). .NET 2.0 must be installed on the target computer system prior to installing *PhaseCalc*. The program is distributed using a Windows Logo compliant [InstallShield](#) setup package. This setup package copies all the necessary files to run the program.

PhaseCalc must be activated before it can be used to perform calculations. Tomcej allows the program to be installed and activated on up to two machines. Additional installations require special licensing arrangements. Please contact Tomcej Engineering if this is the case. Activation is a one-time process that involves sending a machine-specific installation code by e-mail to Tomcej and receiving a license file in return.