

# **ASTEM97**

**Based on the  
IAPWS IF97**

**Water and Steam Properties  
for Industrial Use**

Implementation by

Edward D. Throm (C) 2002 , 2005

**What Is It?  
&  
What's New**

**Version 2.0**



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## Introduction

**ASTEM97, A Steam Table Evaluation Model** based on the IAPWS IF97 release for Water and Steam Properties for Industrial Use (IAPWSa), is a FORTRAN-based dynamic link library (DLL) for the calculation of the thermodynamic properties of water and steam, and for selected additional transport properties:

ID	1-phase	2-phase	Parameter	Sym	SI Units	÷ Conversion =	English Unit
1	✓	✓	Pressure	p	Pa	6.8947570e+03	psia
2	✓	✓	Temperature	T	K	not applicable	°F
3	✓	✓	Specific Volume	v	m <sup>3</sup> /kg	6.2427974e-02	ft <sup>3</sup> /lbm
4	✓	✓	Specific Internal Energy	u	kJ/kg	2.3260000e+00	BTU/lbm
5	✓	✓	Specific Enthalpy	h	kJ/kg	2.3260000e+00	BTU/lbm
6	✓	✓	Specific Entropy	s	kJ/kg-K	4.1868000e+00	BTU/lbm-°F
7	✓	✓	Quality	X	---	1.0000000e+00	---
8	✓		Specific Heat at p=const	C <sub>p</sub>	kJ/kg-k	4.1868000e+00	BTU/lbm-°F
9	✓		Specific Heat at v=const	C <sub>v</sub>	kJ/kg-k	4.1868000e+00	BTU/lbm-°F
10	✓		Sonic Velocity	w	m/sec	3.0480000e-01	ft/sec
11	✓		dv/dp at T=const	(∂v/∂p) <sub>T</sub>	m <sup>3</sup> /kg-Pa	9.0544125e-06	ft <sup>3</sup> /lbm-psi
12	✓		dv/dT at p=const	(∂v/∂T) <sub>p</sub>	m <sup>3</sup> /kg-k	1.1237035e-01	ft <sup>3</sup> /lbm-°F
13	✓		dp/dv at T=const	(∂p/∂v) <sub>T</sub>	Pa-kg/m <sup>3</sup>	1.1044339e+05	psi-lbm/ft <sup>3</sup>
14	✓		dp/dT at v=const	(∂p/∂T) <sub>v</sub>	Pa/K	1.2410563e+04	psi/°F
15	✓		Coef of Thermal Expansion	β	1/K	1.8000000e+00	1/°F
16	✓		Isothermal Compressibility	α	1/Pa	1.4503774e-04	1/psi
17	✓		Isentropic Exponent	κ	---	1.0000000e+00	---
18	✓		Dynamic Viscosity	η	micro kg/m-sec	1.4881640e+06	lbm/ft-sec
19	✓		Surface Tension	σ	milli N/m	1.4593900e+04	lbf/ft
20	✓		Thermal Conductivity (Ind)	k <sub>IND</sub>	W/m-K	1.7307350e+00	BTU/hr-ft-°F
21	✓		Thermal Conductivity (Gsi)	k <sub>GSI</sub>	W/m-K	1.7307350e+00	BTU/hr-ft-°F
22	✓		Refractive Index (λ=1)	n	---	1.0000000e+00	---
23	✓		Static Dielectric Constant	ε	---	1.0000000e+00	---
24	✓	✓	Gibbs Free Energy	g <sub>FE</sub>	kJ/kg	2.3260000e+00	BTU/lbm
25	✓	✓	Helmholtz Free Energy	f <sub>FE</sub>	kJ/kg	2.3260000e+00	BTU/lbm
26	✓		Joule-Thomson Coef	μ <sub>JT</sub>	K/Pa	8.0576524e-05	°F/psi
27	✓		Isothermal Joule-Thom Coef	μ <sub>T</sub>	kJ/kg-Pa	3.3735779e-04	BTU/lbm-psi
28	✓		Kinematic Viscosity	ν	micro m <sup>2</sup> /sec	9.2903040e-02	ft <sup>2</sup> /sec
29	✓	✓	Compressibility Factor	Z	---	1.0000000e+00	---
30	✓		Prandtl Number	Pr	---	1.0000000e+00	---
31	✓	✓	Density	ρ	kg/m <sup>3</sup>	1.6018460e+01	lbm/ft <sup>3</sup>

IAPWS IF-97 (IAPWSa) covers the range:

273.15 K to 1,073.15 K from 611.213 Pa to 100 MPa

and

273.15 K to 2,273.15 K from 611.213 Pa to 10 MPa

**ASTEM97** Version 2.0 includes all IAPWS IF97 releases through July 2005, including:

- IAPWSa Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (September 1997).
- IAPWSg Supplementary Release on Backward Equations for Pressure as a Function of Enthalpy and Entropy  $p(h,s)$  to the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (September 2001).
- IAPWSH 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).
- IAPWSi Supplemental 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).
- IAPWSj 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).

In addition, **ASTEM97** includes transport properties based on the IAPWS releases:

- IAPWSb Release on the IAPS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substance (September 1998)
- IAPWSc1 Release on the IAPS Formulation 1985 for the Viscosity of Ordinary Water Substance (September 1997 )
- IAPWSc2 Revised Release on the IAPS Formulation 1985 for the Viscosity of Ordinary Water Substance (August 2003 )
- IAPWSd Release on the Refractive Index of Ordinary Water Substance as a Function of Wavelength, Temperature and Pressure (September 1997)
- IAPWSe Release on the Static Dielectric Constant of Ordinary Water Substance for Temperatures from 238 K to 873 K and Pressures up to 1000 MPa
- IAPWSf IAPWS Release on Surface Tension of Ordinary Water Substance (September 1994)

## Numerics

Perhaps the most important feature in **ASTEM97** is the numerics used to perform the calculations of the IAPWS equations. **ASTEM97** uses optimized numerics to perform the calculations. Unlike some implementations, **ASTEM97** does not use the summation approach as shown in the following code block:

```
FUNCTION V3ZA(PIN,TIN)
C IAPWS IF-97 FOR WATER AND STEAM CODED BY E.D. THROM (C) 2005
C SPECIFIC VOLUME AT PRESSURE,TEMPERATURE NEW REGION 3 FORMULATIONS
C IAPWS 97 REGION 3 BACKWARD 3Z MODEL A USES SUMMATION AND POWERS
C INPUT      PIN - PRESSURE PA
C           TIN - TEMPERATURE K
C RETURN V3ZPT97B - SPECIFIC VOLUME - M^3/KG
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION IN(23),JN(23),RN(23)
      DATA RN /
X 0.244007892290650D-10 , -0.463057430331242D07 ,
X 0.728803274777712D10 , 0.327776302858856D16 ,
X -0.110598170118409D10 , -0.323899915729957D13 ,
X 0.923814007023245D16 , 0.842250080413712D-12 ,
X 0.663221436245506D12 , -0.167170186672139D15 ,
X 0.253749358701391D04 , -0.819731559610523D-20 ,
X 0.328380587890663D12 , -0.625004791171543D08 ,
X 0.803197957462023D21 , -0.204397011338353D-10 ,
X -0.378391047055938D04 , 0.972876545938620D-2 ,
X 0.154355721681459D02 , -0.373962862928643D04 ,
X -0.682859011374572D11 , -0.248488015614543D-3 ,
X 0.394536049497068D07 /
      DATA IN / -8, -6, -5, -5, -4, -4, -4, -3, -3, -3, -2, -1, 0 ,
1 1, 2, 3, 3, 6, 6, 6, 6, 8, 8 /
      DATA JN/ 3, 6, 6, 8, 5, 6, 8, -2, 5, 6, 2, -6, 3 ,
1 1, 6, -6, -2, -6, -5, -4, -1, -8, -4 /
      PIE = PIN/22.D6 - 0.993D0
      TAU = TIN/650.D0 - 0.994D0
      V3ZA = 0.0D0
      DO 10 I = 1 , 23
10 V3ZA = V3ZA + RN(I)*PIE**IN(I)*TAU**JN(I)
      CONTINUE
      V3ZA = 0.0038D0*V3ZA**4
      RETURN
      END
```

**ASTEM97** optimizes calculations, as shown in the following code block, results is a speed improvement factor of 16 times faster for this function:

```
FUNCTION V3ZB(PIN,TIN)
C IAPWS IF-97 FOR WATER AND STEAM CODED BY E.D. THROM (C) 2005
C SPECIFIC VOLUME AT PRESSURE,TEMPERATURE NEW REGION 3 FORMULATIONS
C IAPWS 97 REGION 3 BACKWARD 3Z MODEL B FASTER BY A FACTOR OF 22 TO 23
C INPUT      PIN - PRESSURE PA
C           TIN - TEMPERATURE K
C RETURN V3ZB - SPECIFIC VOLUME - M^3/KG
      IMPLICIT REAL*8(A-H,O-Z)
      PARAMETER (
X R01 = 0.244007892290650D-10 , R02 = -0.463057430331242D07 ,
X R03 = 0.728803274777712D10 , R04 = 0.327776302858856D16 ,
X R05 = -0.110598170118409D10 , R06 = -0.323899915729957D13 ,
X R07 = 0.923814007023245D16 , R08 = 0.842250080413712D-12 ,
X R09 = 0.663221436245506D12 , R10 = -0.167170186672139D15 ,
X R11 = 0.253749358701391D04 , R12 = -0.819731559610523D-20 ,
X R13 = 0.328380587890663D12 , R14 = -0.625004791171543D08 ,
X R15 = 0.803197957462023D21 , R16 = -0.204397011338353D-10 ,
```

```

X R17 = -0.378391047055938D04 , R18 = 0.972876545938620D-2 ,
X R19 = 0.154355721681459D02 , R20 = -0.373962862928643D04 ,
X R21 = -0.682859011374572D11 , R22 = -0.248488015614543D-3 ,
X R23 = 0.394536049497068D07 )
PIE = PIN/22.D6 - 0.993D0
TAU = TIN/650.D0 - 0.994D0
P1 = 1.0D0/PIE
P2 = P1*P1
PIE3 = PIE*PIE*PIE
T1 = TAU
T2 = T1*T1
T3 = T2*T1
T4 = T2*T2
T5 = T4*T1
T6 = T3*T3
U1 = 1.0D0/TAU
U2 = U1*U1
U4 = U2*U2
V3ZB =
1 P2*(T2*R11+P1*(T5*(R09+T1*R10))+P1*(T5*(R05+T1*(R06+T2*R07)))
2 +P1*(T6*(R03+T2*R04))+P1*(T6*R02+P2*(T3*R01))))+T3*R13
3 +PIE*(T1*R14+PIE*(T6*R15))+P1*U2*((U4*R12+P2*R08))
4 +PIE3*(U2*(R17+U4*R16))+PIE3*(U1*(R21+U2*U1*(R20+U1*(R19+U1*R18)))
5 +PIE*PIE*(U4*(R23+U4*R22)))
V3ZB = V3ZB*V3ZB
V3ZB = 0.0038D0*V3ZB*V3ZB
RETURN
END

```

For reference, the following timing results are provided to compare the summation method to the **ASTEM97** optimized method for some of the high-level routines:

High-Level Routine	Summation Method	ASTEM97 Optimize	Speed Improvement
GIBB1	25.75	0.656	39
GIBB2	35.39	0.755	47
GIBB5	5.23	0.694	7
HELM3	26.36	0.719	37

**Note:** Timing studies done the same PC. Processor speed, available memory, background tasks, etc., will likely impact performance measures. (Test PC: HP Pavilion, 2.66GHz, 512MB, XP-SP1-Home.)

## Version 2.0 Changes

**ASTEM97** Version 2.0 addresses potential issues related to calls to functions with improper input values, or cases where convergence criteria may not be met.

### **ROOT3(p,T, $\rho$ )**

Subroutine ROOT3 computes the density ( $\rho$ ) given the pressure and temperature in IF97 Region 3. This allows the user to maintain consistency with a (p,T) model when in IF97 Region 3. The temperature and density are then used in HELM3 to obtain properties, or in any other temperature and density based routine. **NOTE:** ROOT3 should not be used on the saturation line. ROOT3MAX is provided for calculations on the saturation line. [Ver 2] If the (p,T) input is outside IF97 Region 3, and return value is set to -1.0 and the error code (IERR97(1)) is set to -1.

### **ROOT3MAX(T, $\rho_f$ , $\rho_g$ )**

Subroutine ROOT3MAX returns the saturation fluid density ( $\rho_f$ ) and the saturation vapor density ( $\rho_g$ ) at the input temperature. The temperature and saturation density are then used in HELM3 to obtain saturation properties, or in any other temperature and density based routine to obtain saturation properties. Appendix B provides additional details on ROOT3MAX options and obtaining saturated properties in IF97 Region 3. [Ver 2] This mid-level regional routine does an internal check on the input. The convergence criteria have been updated to fix an, albeit unlikely, internal math error of a divide by zero. In addition if T is less than 623.15 K the error flag is set to -3 and  $\rho_f$  and  $\rho_g$  are set to -1.0, or if T is greater than 647.096 K the error flag is set to -4 and  $\rho_f$  and  $\rho_g$  are set to -1.0.

## Function With Modified Convergence

The convergence criteria used in PVH97 and TVH97 have been relaxed to address a few cases of non-convergence.

The convergence criteria used in PVS97 and TVS97 have been relaxed to address a few cases of non-convergence.

In **Version 2.0**, an iteration counter has been added to the routines identified in the table below. IFLAG97(15) will contain the routine identifier if the number of iterations exceeds a pre-set, large value. No notice is provided as it is likely the solution is converging, just not to the pre-set convergence criterion. After relaxing the convergence criterion for PVH97, TVH97, PVS97 and TVS97, no situation has yet been identified where the iteration failure criterion has been reached. The purpose of adding the counter is to preclude an infinite loop. The value of IFLAG97(15) can be retrieved by a call to IERR97(15) at the end of a problem to verify convergence, with a return value of 0. A check of IFLAG97(15) should be made for any suspect problem.

ASTEM97 Routine	IFLAG97(15) Value
OVHS97	-101
PHS97	-102
PVAR97	-103
PVHS97	-104
ROOT3	-105
ROO3L	-106
ROOTMAX	-107
TVAR97	-108
XREG1MM	-109
XREG1MP	-110
XREG1PM	-111
XREG1PP	-112

### Improved Identification of Saturation Line

IPRS97 has been updated to improve the identification of the saturation line (to return quality of X=0 or X=1) from the **ASTEM97** pressure related functions PTV97, PTU97, PTH97 and PTS97. If the quality falls within  $\pm 1.0 \times 10^{-12}$  of 0 or 1, the input point is identified as being on the saturation line.

### Backward Equations

Functions for IF97 region 3 and IF97 Region 4' (the saturation region with  $s > 5.21$  kJ/kg-K) have also been developed (IAPWS<sub>h</sub> and IAPWS<sub>i</sub>) for T(p,h), T(p,s), p(h,s) and T(h,s), as well as additional functions for v(p,h), v(p,s) and v(h,s) in IF97 Region 3, and for T<sub>sat</sub>(h,s) and x(h,s) in IF97 Region 4' (IAPWS<sub>i</sub>).

The IAPWS T(p,h) backward equations are data fits. To accommodate cases where the resulting temperature returned from these functions is outside the IF97 range (273.15 to 1073.15 K), but still within an acceptable level of "accuracy," **ASTEM97** flag IFLAG97(14) can be set to 1 (for example IRNG = ISET97(14,1)) to force these function to return the minimum or maximum value enabling the user problem to continue to run without violating the IF97 (p,T) range.

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The IAPWS  $p(h,s)$  backward equations are data fits. To accommodate cases where the resulting pressure returned from these functions is outside the IF97 range (611.213 Pa to 100 MPa), but still within an acceptable level of “accuracy,” **ASTEM97** flag IFLAG97(14) can be set to 1 (for example IRNG = ISET97(14,1)) to force these function to return the minimum or maximum value enabling the user problem to continue to run without violating the IF97 (p,T) range.

The IAPWS  $T(h,s)$  backward equations are data fits. To accommodate cases where the resulting temperature returned from these functions is outside the IF97 range ( 273.15 to 1073.15 K), but still within an acceptable level of “accuracy,” **ASTEM97** flag IFLAG97(14) can be set to 1 (for example IRNG = ISET97(14,1)) to force these function to return the minimum or maximum value enabling the user problem to continue to run without violating the IF97 (p,T) range.

In IF97 Region 3, function VR3PT97B(p,T) was added to compute the specific volume given p and T as described in Tables 2 and 10 of IAPWSj. VR3PT97B used functions V3APT97B through V3ZPT97B and TR3PT97B to determine the sub-region containing the specific volume for the input values of p and T. IERR97(1) is set to the sub-region value, 1 to 26 for regions A through Z respectively. If the input temperature is equal to the saturation temperature at p, then IERR97(1) is set to 30 and VR3PT97B return the saturation liquid specific volume and PTMANS97(4) contains the saturation vapor specific volume. If p is less than  $p_{sat}$  at 623.15 K, VR3PT97B returns -1.0 with IERR97(1) set to -1. If p is greater than 100 MPa, VR3PT97B returns -1.0 with IERR97(1) set to -2. If T is less than or equal to 623.15 K, VR3PT97B returns -1.0 with IERR97(1) set to -3. If T is greater than T2397(p), VR3PT97B returns -1.0 with IERR97(1) set to -4.

## Transport Equations

The density based transport equation, for example TC85RHO, takes density and temperature as input, consistent with the IAPWS function development. [Ver 2] The density and temperature are checked. If exceeded, the return value is -1.0 and the error flag is set as described in Appendix A.

TC97PRS. The calculation for  $k_{GSI}$  includes the viscosity adjustment presented in IAPWS<sub>c2</sub> (August 2003 Release) for the dynamic viscosity for general and scientific use, in the range  $0.996 \leq T^* \leq 1.01$  and  $0.71 \leq \rho^* \leq 1.36$ . (In the September 1997 release, IAPWS<sub>c1</sub>, these ranges were:  $0.9970 \leq T^* \leq 1.0082$  and  $0.775 \leq \rho^* \leq 1.290$ .) In **ASTEM97**, the dynamic viscosity is obtained for the industrial use formulation.

## ASTEM97MC Bug Fix

In the **ASTEM97** Mathcad® version, **ASTEM97MC**, a bug in function *iprs97mc* has been fixed. If the default units are set to English, calling *iprs97mc* with pressure and specific volume had an error. The internal conversion of the specific volume to SI units used the conversion for density instead of specific volume.