ASTEM97

Based on the
IAPWS IF-97

Water and Steam Properties
for Industrial Use

Implementation by

Edward D. Throm

Appendix C

Near the
Critical Point

Table of Contents

List of Figures

Introduction

Near the critical point, 22.064 MPa and 647.096 K, the IAPWS correlation for the thermal conductivity for general and scientific use (K_{GSI}) and for the specific heat capacity (C_p) both exhibit some numerical problems. Studies performed with temperature steps of 1.0×10^{-8} and 1.0×10^{-7} K have been performed to determine the scope of the problems. Based on these results, a minimum ΔT of 1.0×10^{-7} K is recommended for general use in **ASTEM97**.

Specific Heat Capacity (C_p)

The equation for the specific (isobaric) heat capacity (C_p), or the heat capacity at constant pressure, exhibits numerical inconsistences near the critical point. At the critical point, 22.064 MPa and 647.096 K, the value computed with the dimensionless Helmholtz free energy and its derivatives is -771,622,364,815.17 kJ/kg-K, a negative values. Figure 1 demonstrates this characteristic at a pressure of 22.064 MPa.

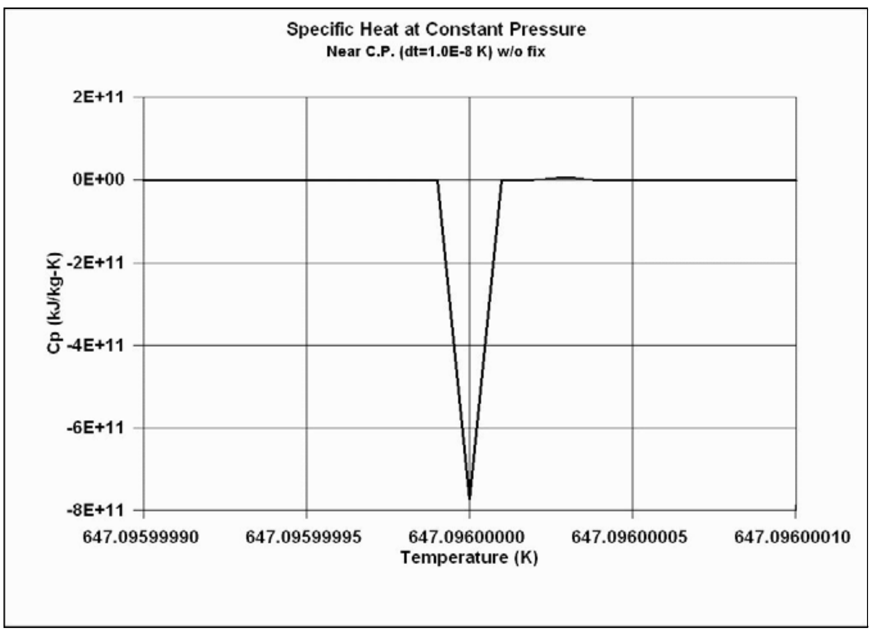

Figure 1 - C_p near critical point without ASTEM97 fix

To “fix” this problem, a user flag is available which will decrease the user provided pressure in steps of 1.0×10^{-7} Pa until a positive value is calculated. The user sets a flag (number 6) with the ISET97 function, for example IFIX = ISET97(6,1). Figure 2 demonstrates the results with the flag set, again at a pressure of 22.064 MPa. A ΔT of 1.0×10^{-8} K was used to develop the plot. The peak value does not occur at 647.096 K and shows some “erratic” behavior.

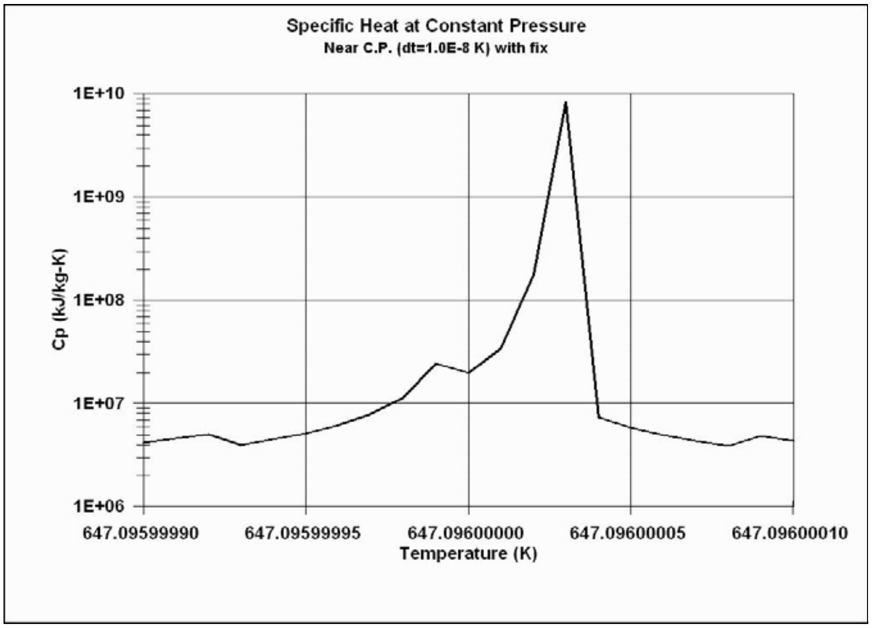

Figure 2 - C_p near critical point, ΔT=1.0x10^{-8} K with fix

In **ASTEM97**, it is recommended that a ΔT of 1.0x10^{-7} K be used. Figure 3 presents the expected results for C_p near the critical point when using this value.

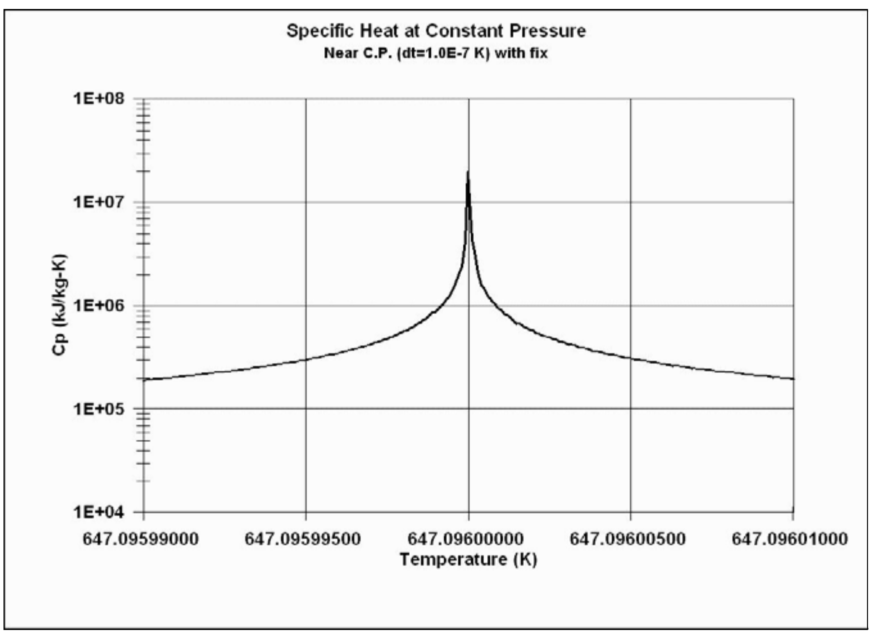

Figure 3 - C_p near critical point, ΔT=1.0x10^{-7} K with fix

Thermal Conductivity (k)

Near the critical point, the correlation for k_{GSI} returns a negative value for the dimensionless partial derivative $(\partial\delta/\partial\pi)|_\tau$ (see Equation 22 in IAPWSb, Appendix C) which is raised to a negative value. The result is an undefined value. To account for this problem, if $(\partial\delta/\partial\pi)|_\tau$ is calculated to be negative, $(\partial\delta/\partial\pi)|_\tau$ is set to $1.0\text{x}10^{-4}$, a small number. This value was chosen for **ASTEM97** based on a review of the Prandtl number. The resulting value for the Prandtl number at the critical point as compared to the values at ± $1.0\text{x}10^{-7}$ K has about the same ratio as the Prandtl number computed with k_{IND} (for industrial use), as shown below:

```
Dv-IND - dynamic viscosity w/o adjustment, Dv-GSi - with adjustment
Tc-IND - thermal conductivity without adjustment, Tc-GSI - with adjustment
Pr-GSI = 1000.*Cp*DV-GSI/Tc-GSI, Pr-IND = 1000.*Cp*DV-IND/Tc-85
```

P	T	Cp	Dv-IND	Dv-GSI	Tc-IND	Tc-GSI	Tc-85	Pr-GSI	Pr-IND
MPa	K	kJ/kg-K	µkg/m-s	µkg/m-s	W/m-K	W/m-K	W/m-K	---	---
22.064	647.0959999	4.1852e+06	39.497	51.784	30.612	23.396	0.8107	9.264e+09	2.039e+11
22.064	647.0960000	1.9658e+07	39.430	51.787	31.639	24.137	0.8106	3.211e+10	9.562e+11
22.064	647.0960001	4.3560e+06	39.365	51.654	31.201	23.824	0.8104	9.444e+09	2.116e+11

Figure 4 demonstrates the results with the above modification, or fix in **ASTEM97**, at a pressure of 22.064 MPa. A ΔT of $1.0\text{x}10^{-8}$ K was used to develop the plot. The peak value does not occur at 647.096 K and shows some "erratic" behavior.

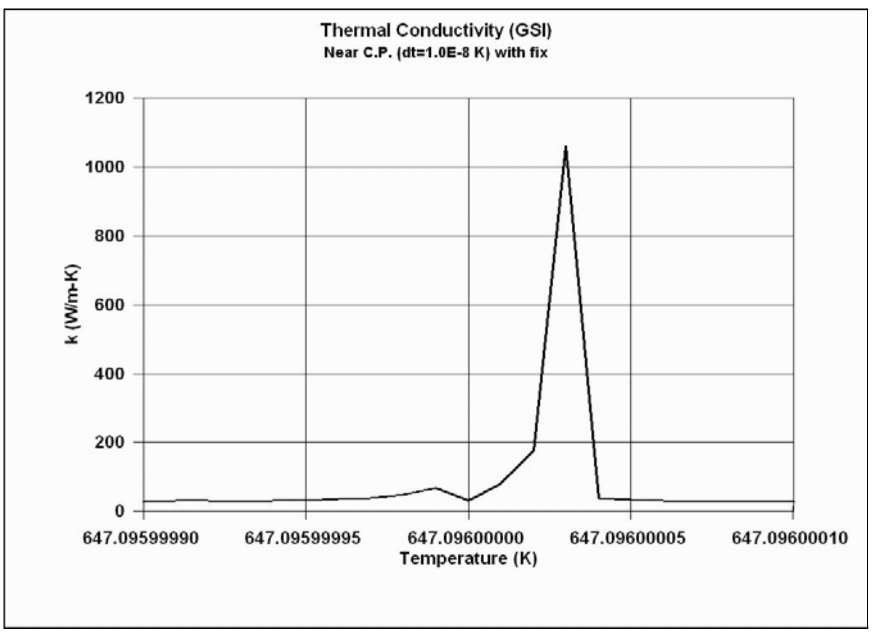

Figure 4 - k_{GSI} near critical point, ΔT=$1.0\text{x}10^{-8}$ K with fix

In **ASTEM97**, it is recommended that a ΔT of $1.0\text{x}10^{-7}$ K be used. Figure 5 presents the expected results for k_{GSI} near the critical point when using this value.

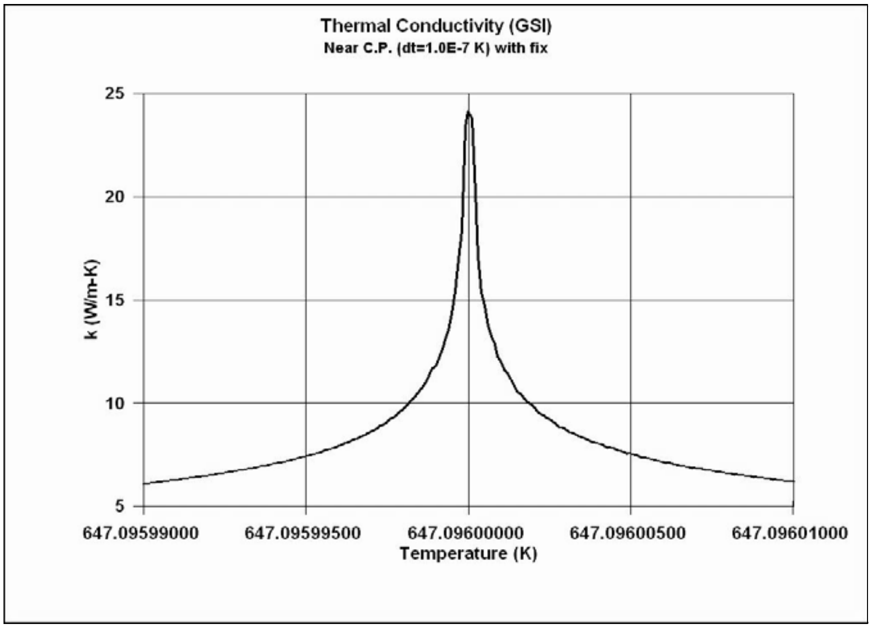

Figure 5 - k_{GSI} near critical point, $\Delta T=1.0x10^{-7}$ K with fix

For comparison, k_{IND} is shown in Figure 6.

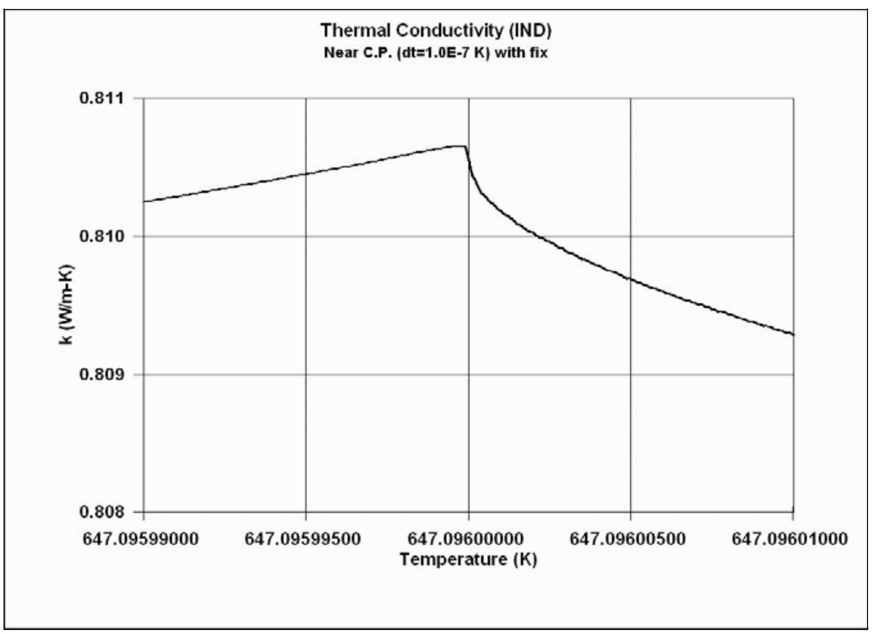

Figure 6 - k_{IND} near critical point, $\Delta T=1.0x10^{-7}$ K

Prandtl Number (Pr)

The Prandtl number results based on using C_p with the **ASTEM97** fix near the critical point and k_{GSI} (as modified, or fixed, in **ASTEM97**) or k_{IND} are shown in Figure 7.

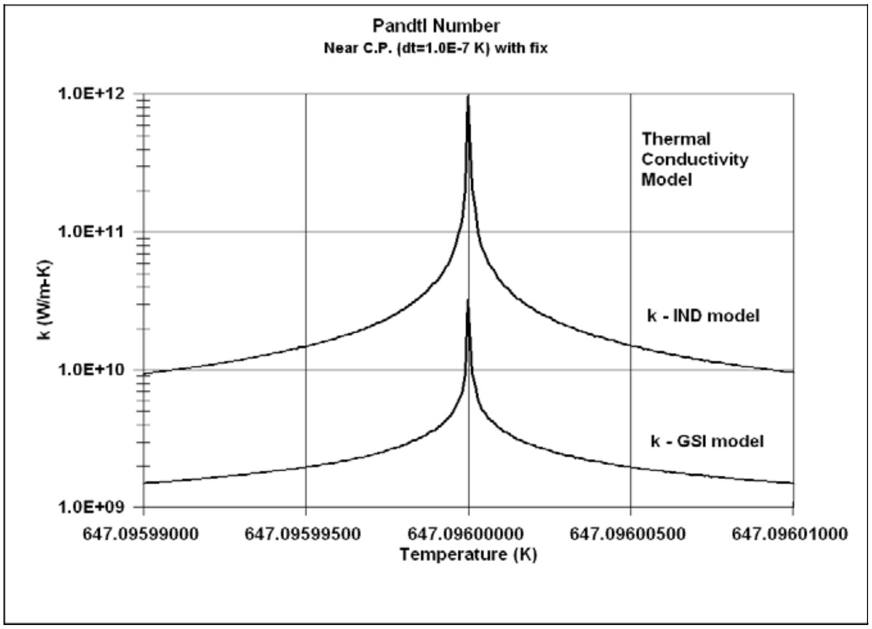

Figure 7 - Prandtl number (Pr) based on k_{GSI} and k_{IND}

Reference:

IAPWSb Release Release on the IAPS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substance (September 1998)