CADET ____________________ SECTION ______ TIME OF DEPARTURE ________

DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2023-2024
Veteran's Day Bonus
31 October 2023

TEXT: Smith, Van Ness, & Abbott
SCOPE: Lessons 22-32
ANTICIPATED TIME: 60 Minutes

References Permitted: Open notes, book, internet, CHEMCAD, Mathematica, Excel.

INSTRUCTIONS

1. This is a BONUS exercise and is due **1630 13 November 2023**.
2. There are 2 problems on three pages (not including the cover or reference pages).
3. A Mathematica file "VDB_Gibbs_Generating_Function.nb" that accompanies this handout is found in Canvas.
4. The reference article "VDB_Reference_Article_IF97.pdf" that accompanies this handout is found in Canvas.
5. A Microsoft Word file "VDB_Deliverables.docx" that accompanies this handout is found in Canvas.
6. Deliverables are your completed tables and Mathematica files in pdf format with cover sheet in a single pdf file, plus working Mathematica and CHEMCAD files (three files total). Save all electronic work in Canvas.

(TOTAL WEIGHT: 30 POINTS)

DO NOT WRITE IN THIS SPACE

PROBLEM	VALUE	ADD
A	15	
B	15	
TOTAL BONUS	30	

Cadet:________________________

Problem: Weight:
A 15

In Lesson 27, we discussed the idea that the Gibbs energy function is a generating function for all other thermodynamic properties. The steam tables are an important application of this principle.[1] The properties in the tables are calculated from the Gibbs energy according to the generating functions in Table 1.

Table 1. Thermodynamic property relations derived from the Gibbs energy function (equation 1) and its derivatives.

Property	Relation	Reference
Specific Volume	$v=\left(\partial g/\partial p\right)_T$	L27, Slide 11
Specific Internal energy	$u=g-T\left(\partial g/\partial T\right)_p-P\left(\partial g/\partial p\right)_T$	Eq. 6.1 (L27 Slide 6), combined with definitions of specific entropy and volume (*s* and *v*).
Specific entropy	$s=-\left(\partial g/\partial T\right)_p$	L27, Slide 11
Specific enthalpy	$h=g-T\left(\partial g/\partial T\right)_p$	Eq 6.4 (L27 Slide 6), combined with above definition of specific entropy *s*.

The Gibbs energy generating function for steam is

$$\frac{g(T,p)}{RT}=\sum_{i=1}^{34} n_i\left(7.1-\pi\right)^{I_i}\left(\tau-1.222\right)^{J_i} \tag{1}$$

where $\pi = p/p^*$, $\tau = T^*/T$, $p^* = 16.53$ MPa, $T^* = 1386$ K and $R = 0.461526$ kJ kg^{-1} K^{-1}. The constants n_i, I_i, and J_i, as well an implementation of equation 1, are included in the Mathematica file that accompanies this exercise. [2]

In this assignment, you will modify the provided Mathematica file to calculate *v*, *u*, *s*, and *h* using the property relations in Table 1. To receive any credit, you must verify the test values in Table 2 on the following page. Ensure that your calculated answers contain the same precision as shown in Table 2 (nine significant figures), and <u>complete Table 3</u> using your Mathematica results using the same format as in Table 2.

Table 2. Thermodynamic property values calculated using equation 1 for selected values of T and p.

Property	T = 300 K p = 3 MPa	T = 300 K p = 80 MPa	T = 500 K p = 3 MPa
v / (m^3 kg^{-1})	0.100 215 168 × 10^{-2}	0.971 180 894 × 10^{-3}	0.120 241 800 × 10^{-2}
h / (kJ kg^{-1})	0.115 331 273 × 10^3	0.184 142 828 × 10^3	0.975 542 239 × 10^3
u / (kJ kg^{-1})	0.112 324 818 × 10^3	0.106 448 356 × 10^3	0.971 934 985 × 10^3
s / (kJ kg^{-1} K^{-1})	0.392 294 792	0.368 563 852	0.258 041 912 × 10^1

The format of the entries in this table follow Table 5 in Reference 1.

Table 3. Cadet MATHEMATICA answers for comparison with Table 2.

Property	T = 300 K p = 3 MPa	T = 300 K p = 80 MPa	T = 500 K p = 3 MPa
v / (m^3 kg^{-1})			
h / (kJ kg^{-1})			
u / (kJ kg^{-1})			
s / (kJ kg^{-1} K^{-1})			

Note: Cadets should use the same format for numbers as in Table 2.

Cadet:________________________

Problem:	Weight:
B	15

Design a CHEMCAD flow sheet that allows you to calculate *v*, *s*, *u*, and *h* and compare your answers to the values in Table 2. Complete Table 4 using *nine* significant figures and in the same format used in Table 2.

Table 4. Cadet CHEMCAD answers for comparison with Table 2.

Property	T = 300 K p = 3 MPa	T = 300 K p = 80 MPa	T = 500 K p = 3 MPa
v / (m^3 kg^{-1})			
h / (kJ kg^{-1})			
u / (kJ kg^{-1})			
s / (kJ kg^{-1} K^{-1})			

Note: Cadets should use the same format for numbers as in Table 2.

References

1. The calculations in this exercise are found in IAPWS R7-97(2012), published by the International Association for the Properties of Water and Steam, Lucerne, Switzerland, August 2007. IAPWS R7-97(2012) is widely used in process simulators such as CHEMCAD and has been standardized by international convention.

2. The Gibbs energy function and the constants in this document pertain to Region 1 in Reference 1. Specifically, region 1 is $273.15 < T < 623.15$ K and $p^{sat}(T) < p < 100$ MPa. Other constants in Reference 1 pertain to other temperature-pressure regions.