CADET _____ SECTION _____ TIME OF DEPARTURE _____

## DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2024-2025                    TEXT: Smith, Van Ness, & Abbott
WRITTEN PARTIAL REVIEW III         SCOPE: Lessons 22-32
20 November 2024, A-Hour           TIME: 55 Minutes

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

### INSTRUCTIONS

1. Do not mark this exam or open it until "begin work" is given.
2. You have 55 minutes to complete the exam.
3. There are 3 problems on 3 pages in this exam (not including the cover page). Write your name on the top of each sheet.
4. Solve the problems in the space provided and in Mathematica. Show all work to receive full credit.
5. Laptops are authorized for referencing only. Desktop PCs must be used for all calculations.
6. Save Mathematica and CHEMCAD files on your desktop and re-save frequently.
7. When finished, upload all electronic work files to Canvas.


(TOTAL WEIGHT: 200 POINTS)
_____


DO NOT WRITE IN THIS SPACE

| PROBLEM | VALUE | CUT |
|---------|-------|-----|
| A | 40 | |
| B | 100 | |
| C | 60 | |
| TOTAL CUT | | |
| TOTAL GRADE | 200 | |

Problem:    Weight:
  A            40

Use Table C.1 on page 669 of the textbook with gas constant R=8.314 J/(mol·K) to calculate $\Delta H^{ig}$ and $\Delta S^{ig}$ for *ideal* gas-phase methane compressed and heated from 298.15 K and 1 bar to 500.0 K and 50.00 bar. Report your answers for $\Delta H^{ig}$ and $\Delta S^{ig}$ in J/mol and J/(mol·K), respectively.

**Solution:**

```
(*Methane*)
p = 50.00; (*bar*)
t = 500.0; (*K*)

R = 8.314; (*J/(mol*K)*)

a = 1.702;
b = 9.081 * 10^-3;
c = -2.164 * 10^-6;
Cp = a + b * T + c * T^2;

(*enthalpy*)
Hig = R * ∫²⁹⁸.¹⁵ᵗ Cp dT (*eq 2.21*)
```

$$Hig = R * \int_{298.15}^{t} Cp \, dT \quad (*eq\ 2.21*)$$

```
(*entropy*)
```

$$Sig = R * \left( \int_{298.15}^{t} \frac{Cp}{T} \, dT - Log\left[\frac{p}{1}\right] \right) \quad (*eq\ 5.10*)$$

Out[17]= <u>8347.29224731</u>  J/mol
                    ANS, $\Delta H_{ig}$

Out[18]= <u>-11.4183403666</u>  J/(mol·K)
                    ANS, $\Delta S_{ig}$

Problem:    Weight:
   B            100

Use the SRK equation of state to calculate the compressibility, residual enthalpy, and residual entropy ($Z$, $H^R$, and $S^R$) for methane at 500.0 K and 50.00 bar.

Use Table B.1 on pages 663-665 of the textbook for critical constants and acentric factor. Use gas constant R=8.314 J/(mol·K). Report your answers for $H^R$ and $S^R$ in J/mol and J/(mol·K), respectively.

**Solution:**

```
(*Methane, Table B.1, p.663*)
tc = 190.6; (*K*)
pc = 45.99; (*bar*)
ω = 0.012;

(*Reduced t and p*)
tr = t / tc;  pr = p / pc;

(*Table 3.1 page 100*)
σ = 1; ε = 0; Ω = 0.08664; Ψ = 0.42748;
α[x_] = (1 + (0.480 + 1.574 * ω - 0.176 * ω²) * (1 - √x))²;
```

$$\text{In[78]:= } \beta = \Omega * pr / tr; \quad (*eq\ 3.50*)$$

$$q[x\_] = \Psi * \alpha[x] / (\Omega * x); \quad (*eq\ 3.51*)$$

$$eq1 = z == 1 + \beta - q[tr] * \beta * \frac{z - \beta}{(z + \epsilon * \beta) * (z + \sigma * \beta)}; \quad (*eq\ 3.48*)$$

$$Z = z /. \text{Quiet}[\text{Solve}[eq1, z, \text{Reals}]]\llbracket 1 \rrbracket;$$

$$I = \frac{1}{\sigma - \epsilon} * \text{Log}\left[\frac{Z + \sigma * \beta}{Z + \epsilon * \beta}\right]; \quad (*eq\ 13.72*)$$

$$Hr[x\_] = (Z - 1 + x * \partial_x q[x] * I) * R * t; \quad (*13.75*)$$

$$Sr[x\_] = (\text{Log}[Z - \beta] + (q[x] + x * \partial_x q[x]) * I) * R; \quad (*13.76*)$$

```
In[85]:= Z
         Hr[tr]
         Sr[tr]
```

Out[85]= 1.00607478317
                          ‾‾‾‾‾‾‾‾‾‾ ANS, Z

Out[86]= −258.671254362 J/mol
                          ‾‾‾‾‾‾‾‾‾‾ ANS, $S^R$

Out[87]= −0.557907268858 J/(mol·K)
                          ‾‾‾‾‾‾‾‾‾‾ ANS, $H^R$

Problem: Weight:
  C      60

(a) Using the results in the table below with standard heats of formation from Table C.4 on pages 671-672 of the textbook, calculate the total real-gas enthalpy and entropy of methane at 500.0 K and 50.00 bar. Report your answers for H and S in J/mol and J/(mol·K), respectively.

|  | Ideal | Residual | Total |
|---|---|---|---|
| Enthalpy, J/mol | 8,347.292 | -258.671 | -66,431.379 //ANS |
| Entropy, J/mol·K | -11.418 | -0.558 | -92.674 //ANS |

(b) Use CHEMCAD and the CHEMCAD file in Canvas to calculate the enthalpy and entropy of methane at 500.0 K and 50.00 bar using the SRK equation of state and complete the following table:

| | |
|---|---|
| CHEMCAD Enthalpy, J/mol | -66,882  //ANS |
| CHEMCAD Entropy, J/mol·K | -92.76  //ANS |

(c) Give two reasons for the differences between the answers in parts (a) and (b).

**Solution, part (a):**

In[98]:= (*Methane, Table C.4, p.671*)
     ΔHfo = -74 520;
     ΔGfo = -50 460;
$$\Delta Sfo = \frac{\Delta Hfo - \Delta Gfo}{298.15};$$

     H = ΔHfo + Hig + Hr[tr] (*6.50*)
     S = ΔSfo + Sig + Sr[tr] (*6.51*)
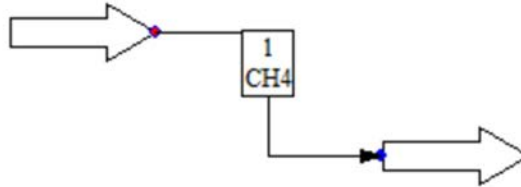
Out[101]= -66 431.3790071  J/mol //ANS
                ANS, H
Out[102]= -92.6738830539  J/(mol·K) //ANS
                ANS, S

**Solution, part (b):**

| Stream No. | 1 |
|---|---|
| Name | CH4 |
| - - Overall - - | |
| Temp K | 500.0000 |
| Pres bar | 50.0000 |
| Enth J/sec | -66882.//ANS |
| Molar flow mol/sec | 1.0000 |
| Entropy    J/K/sec | -92.76//ANS |
| | |

**Solution, part (c):**

The answers are different because of the following: (1) different heat capacity polynomial, (2) different $T_c$, $P_c$, and $\omega$, and (3) different numerical methods. //ANS

CADET _____ SECTION _____ TIME OF DEPARTURE _____

## DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2024-2025                     TEXT: Smith, Van Ness, & Abbott
WRITTEN PARTIAL REVIEW III          SCOPE: Lessons 22-32
20 November 2024, C-Hour            TIME: 55 Minutes

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

### INSTRUCTIONS

1. Do not mark this exam or open it until "begin work" is given.
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6. Save Mathematica and CHEMCAD files on your desktop and re-save frequently.
7. When finished, upload all electronic work files to Canvas.


(TOTAL WEIGHT: 200 POINTS)
_____


DO NOT WRITE IN THIS SPACE

| PROBLEM | VALUE | CUT |
|---------|-------|-----|
| A | 40 | |
| B | 100 | |
| C | 60 | |
| TOTAL CUT | | |
| TOTAL GRADE | 200 | |

Problem:     Weight:
  A              40

Use Table C.1 on page 669 of the textbook with gas constant R=8.314 J/(mol·K) to calculate $\Delta H^{ig}$ and $\Delta S^{ig}$ for *ideal* gas-phase ethane compressed and heated from 298.15 K and 1 bar to 1000.0 K and 100.00 bar. Report your answers for $\Delta H^{ig}$ and $\Delta S^{ig}$ in J/mol and J/(mol·K), respectively.

**Solution:**

```
In[1]:= (*Ethane*)
        p = 100.00; (*bar*)
        t = 1000.0; (*K*)

        R = 8.314; (*J/(mol*K)*)

        a = 1.131;
        b = 19.225 * 10^-3;
        c = -5.561 * 10^-6;
        Cp = a + b * T + c * T^2;

        (*enthalpy*)
```

$$Hig = R * \int_{298.15}^{t} Cp \, dT \; (*eq \; 2.21*)$$

```
        (*entropy*)
```

$$Sig = R * \left( \int_{298.15}^{t} \frac{Cp}{T} \, dT - Log\left[\frac{p}{1}\right] \right) \; (*eq \; 5.10*)$$

Out[8]= 64 410.7732742   J/mol
        _____
                         ANS, $\Delta H_{ig}$

Out[9]= 64.2111300831   J/(mol·K)
        _____
                        ANS, $\Delta S_{ig}$

CH365, AY24-25                    1
WPRIII, C-Hour, Solution

Problem:    Weight:
   B           100

Use the SRK equation of state to calculate the compressibility, residual enthalpy, and residual entropy ($Z$, $H^R$, and $S^R$) for ethane at 1000.0 K and 100.00 bar.

Use Table B.1 on pages 663-665 of the textbook for critical constants and acentric factor. Use gas constant R=8.314 J/(mol·K). Report your answers for $H^R$ and $S^R$ in J/mol and J/(mol·K), respectively.

**Solution:**

```
(*Ethane, Table B.1, p.663*)
tc = 305.3; (*K*)
pc = 48.72; (*bar*)
ω = 0.100;

(*Reduced t and p*)
tr = t / tc;  pr = p / pc;

(*Table 3.1 page 100*)
σ = 1;  ε = 0;  Ω = 0.08664;  Ψ = 0.42748;
α[x_] = (1 + (0.480 + 1.574 * ω - 0.176 * ω²) * (1 - √x))²;
```

```
In[18]:= β = Ω * pr / tr; (*eq 3.50*)
q[x_] = Ψ * α[x] / (Ω * x); (*eq 3.51*)
                                    z - β
eq1 = z == 1 + β - q[tr] * β * ─────────────────────── ; (*eq 3.48*)
                               (z + ε * β) * (z + σ * β)
Z = z /. Quiet[Solve[eq1, z, Reals]][[1]];
      1         ⎡ Z + σ * β ⎤
I = ───── * Log ⎢ ───────── ⎥ ;  (*eq 13.72*)
    σ - ε       ⎣ Z + ε * β ⎦
Hr[x_] = (Z - 1 + x * ∂ₓq[x] * I) * R * t; (*13.75*)
Sr[x_] = (Log[Z - β] + (q[x] + x * ∂ₓq[x]) * I) * R; (*13.76*)
```

```
In[25]:= Z
Hr[tr]
Sr[tr]
```

Out[25]= 1.03757874347
                          ANS, Z

Out[26]= -194.532667476  J/mol
                          ANS, $S^R$

Out[27]= -0.496693158026  J/(mol·K)
                           ANS, $H^R$

Cadet:_____

Problem:    Weight:
  C           60

(a) Using the results in the table below with standard heats of formation from Table C.4 on pages 671-672 of the textbook, calculate the total real-gas enthalpy and entropy of ethane at 1000.0 K and 100.00 bar. Report your answers for H and S in J/mol and J/(mol·K), respectively.

|  | Ideal | Residual | Total |
|---|---|---|---|
| Enthalpy, J/mol | 64,410.773 | -194.533 | -19,603.759 //ANS |
| Entropy, J/mol·K | 64.211 | -0.497 | -110.577 //ANS |

(b) Use CHEMCAD and the CHEMCAD file in Canvas to calculate the enthalpy and entropy of ethane at 1000.0 K and 100.00 bar using the SRK equation of state and complete the following table:

| CHEMCAD Enthalpy, J/mol | -19,601  //ANS |
|---|---|
| CHEMCAD Entropy, J/mol·K | -110.3    //ANS |

(c) Give two reasons for the differences between the answers in parts (a) and (b).

**Solution, part (a):**

(\*Ethane, Table C.4, p.671\*)
$\Delta Hfo = -83\,820;$
$\Delta Gfo = -31\,855;$
$\Delta Sfo = \dfrac{\Delta Hfo - \Delta Gfo}{298.15};$

$H = \Delta Hfo + Hig + Hr[tr]$ (\*6.50\*)
$S = \Delta Sfo + Sig + Sr[tr]$ (\*6.51\*)

Out[31]= $-19\,603.7593933$  J/mol //ANS
                                 ANS, H
Out[32]= $-110.577027103$  J/(mol·K) //ANS
                                  ANS, S

CH365, AY24-25                        3
WPRIII, C-Hour, Solution

Cadet:_____

## Solution, part (b):

| Stream No. | 2 |
|---|---|
| Name | C2H6 |
| - - Overall - - | |
| Temp K | 1000.0000 |
| Pres bar | 100.0000 |
| Enth J/sec | -19601. //ANS |
| Molar flow mol/sec | 1.0000 |
| Entropy     J/K/sec | -110.3 //ANS |
| | |
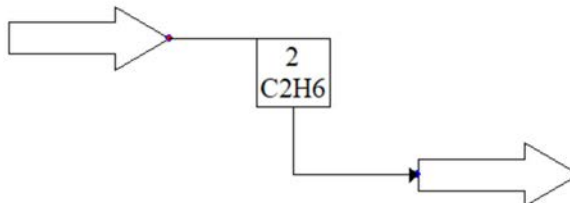
## Solution, part (c):

The answers are different because of the following: (1) different heat capacity polynomial, (2) different $T_c$, $P_c$, and $\omega$, and (3) different numerical methods. //ANS

CADET _____ SECTION _____ TIME OF DEPARTURE _____

DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2024-2025                              TEXT: Smith, Van Ness, & Abbott
WRITTEN PARTIAL REVIEW III          SCOPE: Lessons 22-32
18 November 2024, Make-Ahead        TIME: 55 Minutes

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

## INSTRUCTIONS

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_____

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| PROBLEM | VALUE | CUT |
|---------|-------|-----|
| A | 40 | |
| B | 100 | |
| C | 60 | |
| TOTAL CUT | | |
| TOTAL GRADE | 200 | |

Cadet:_____

Problem:   Weight:
  A          40

Use Table C.1 on page 669 of the textbook with gas constant R=8.314 J/(mol·K) to calculate $\Delta H^{ig}$ and $\Delta S^{ig}$ for *ideal* gas-phase propane compressed and heated from 298.15 K and 1 bar to 400.0 K and 60.00 bar. Report your answers for $\Delta H^{ig}$ and $\Delta S^{ig}$ in J/mol and J/(mol·K), respectively.

**Solution:**

In[1]:=  (*Propane*)
        p = 60.00; (*bar*)
        t = 400.0; (*K*)

        R = 8.314; (*J/(mol*K)*)

        a = 1.213;
        b = 28.785 * 10$^{-3}$;
        c = -8.824 * 10$^{-6}$;
        Cp = a + b * T + c * T$^2$;

        (*enthalpy*)
        Hig = R * $\int_{298.15}^{t}$ Cp dT (*eq 2.21*)

        (*entropy*)
        Sig = R * $\left( \int_{298.15}^{t} \frac{Cp}{T} dT - Log\left[\frac{p}{1}\right] \right)$ (*eq 5.10*)

Out[8]= 8618.75780736  J/mol
        _____  ANS, $\Delta H_{ig}$

Out[9]= -9.31045663582  J/(mol·K)
        _____  ANS, $\Delta S_{ig}$

Cadet:_____

Problem:   Weight:
  B            100

Use the PR equation of state to calculate the compressibility, residual enthalpy, and residual entropy (Z, H$^R$, and S$^R$) for propane at 400.0 K and 60.00 bar.

Use Table B.1 on pages 663-665 of the textbook for critical constants and acentric factor. Use gas constant R=8.314 J/(mol·K). Report your answers for H$^R$ and S$^R$ in J/mol and J/(mol·K), respectively.

**Solution:**

```
In[12]:=  (*Propane, Table B.1, p.663*)
          tc = 369.8; (*K*)
          pc = 42.48; (*bar*)
          ω = 0.152;

          (*Reduced t and p*)
          tr = t / tc;  pr = p / pc;

          (*Table 3.1 page 100*)
          σ = 1 + √2 ;  ε = 1 - √2 ;  Ω = 0.07780;  Ψ = 0.45724;
          α[x_] = (1 + (0.37464 + 1.54226 * ω - 0.26992 * ω²) * (1 - √x ))²;

In[18]:=  β = Ω * pr / tr; (*eq 3.50*)
          q[x_] = Ψ * α[x] / (Ω * x); (*eq 3.51*)
                                      z - β
          eq1 = z == 1 + β - q[tr] * β * ─────────────────────── ; (*eq 3.48*)
                                      (z + ε * β) * (z + σ * β)
          Z = z /. Quiet[Solve[eq1, z, Reals]][[1]];
                1         Z + σ * β
          I = ───── * Log[─────────] ;  (*eq 13.72*)
              σ - ε       Z + ε * β
          Hr[x_] = (Z - 1 + x * ∂ₓq[x] * I) * R * t ; (*13.75*)
          Sr[x_] = (Log[Z - β] + (q[x] + x * ∂ₓq[x]) * I) * R ; (*13.76*)

In[25]:=  Z
          Hr[tr]
          Sr[tr]

Out[25]= 0.466806210657
                            ANS, Z
Out[26]= -6936.59864159   J/mol
                            ANS, S$^R$
Out[27]= -13.4236976404   J/(mol·K)
                            ANS, H$^R$
```

Cadet:_____

Problem:    Weight:
   C           60

(a) Using the results in the table below with standard heats of formation from Table C.4 on pages 671-672 of the textbook, calculate the total real-gas enthalpy and entropy of propane at 400.0 K and 60.00 bar. Report your answers for H and S in J/mol and J/(mol·K), respectively.

|  | Ideal | Residual | Total |
|---|---|---|---|
| Enthalpy, J/mol | 8,618.758 | -6,936.599 | -102,997.841 //ANS |
| Entropy, J/mol·K | -9.310 | -13.424 | -292.364 //ANS |

(b) Use CHEMCAD and the CHEMCAD file in Canvas to calculate the enthalpy and entropy of propane at 400.0 K and 60.00 bar using the PR equation of state and complete the following table:

| CHEMCAD Enthalpy, J/mol | -103,000 //ANS |
|---|---|
| CHEMCAD Entropy, J/mol·K | -291.9 //ANS |

(c) Give two reasons for the differences between the answers in parts (a) and (b).

**Solution, part (a):**

In[28]:= (*Propane, Table C.4, p.671*)
    ΔHfo = -104 680;
    ΔGfo = -24 290;
    ΔSfo = $\frac{\text{ΔHfo} - \text{ΔGfo}}{298.15}$;

    H = ΔHfo + Hig + Hr[tr] (*6.50*)
    S = ΔSfo + Sig + Sr[tr] (*6.51*)

Out[31]= -102 997.840834    J/mol //ANS
                                    ANS, H
Out[32]= -292.36353546    J/(mol·K) //ANS
                                    ANS, S

Cadet:_____

**Solution, part (b):**

| Stream No. | 1 |
|---|---|
| Name | CH4 |
| - - Overall - - | |
| Temp K | 500.0000 |
| Pres bar | 50.0000 |
| Enth J/sec | -66882.//ANS |
| Molar flow mol/sec | 1.0000 |
| Entropy    J/K/sec | -92.76//ANS |
| | |



**Solution, part (c):**

The answers are different because of the following: (1) different heat capacity polynomial, (2) different $T_c$, $P_c$, and $\omega$, and (3) different numerical methods. //ANS