1.) Use ASPEN Properties to calculate the constant pressure heat capacity \((C_p)\) of nitrogen at 55 bar from 100-200 K. Show your results as a plot of \(C_p\) versus temperature. Compare this to data found on the web at http://webbook.nist.gov/chemistry/fluid/

2.) For the air compressor problem done in class (see below), compute the outlet temperature and work done by the compressor by hand. Show all relevant calculations and equations (balances, property relationships, etc.). You may treat the air as an ideal gas with a \(C_p\) of 29.3 J/mol/K. Compare this answer to the one obtained during class.

3.) Generate a \(P-x-y\) diagram for the binary system n-hexane and nitroethane at 45°C. For a vapor mole fraction of 0.8 for n-hexane, what is the equilibrium liquid mole fraction of n-hexane? What is the equilibrium pressure for this two-phase system?

4.) Redo the FLASH simulation of propane and n-butane that was done in class (see below). This time, DO NOT assume IDEAL behavior (that is, do not choose the IDEAL method to represent the thermodynamic properties of the vapor and liquid phases). What property method do you choose instead? What pressure is required to produce equal molar flow rates of vapor and liquid coming from the flash separator? What are the mole fractions of propane and n-butane in the liquid and vapor phases respectively? Compare these results to those obtained using the IDEAL method. Which approach is the best (IDEAL or the one you chose instead)? How can you tell?
Prob 1

Graph showing CP vs Temperature for VAPOR N2 and LIQUID N2.
ILLUSTRATION 2.5-4
Example of a Thermodynamics Problem That Cannot Be Solved With Only the Mass and Energy Balances

A compressor is a gas pumping device that takes in gas at low pressure and discharges it at a higher pressure. Since this process occurs quickly compared to heat transfer, it is usually assumed to be adiabatic; that is, there is no heat transfer to or from the gas during its compression. Assuming that the inlet to the compressor is air (which we will take to be an ideal gas with $C_p = 29.3 \text{ J/(mol K)}$ at 1 bar and 290 K and that the discharge is at a pressure of 10 bar, estimate

a. The temperature of the exit gas
b. The rate at which work is done on the gas (i.e., the power requirement) for a gas flow of 2.5 mol/s.

SOLUTION

The system will be taken to be the gas contained in the compressor. The differential form of the molar mass and energy balances for this open system are

$$\frac{dN}{dt} = \dot{N}_1 + \dot{N}_2$$

$$\frac{dU}{dt} = \dot{N}_1 H_1 + \dot{N}_2 H_2 + \dot{Q} + \dot{W}$$

where we have used the subscripts 1 to indicate the flow stream into the compressor and 2 to indicate the flow stream out of the compressor.

Since the compressor operates continuously, the process may be assumed to be in a steady state,

$$\frac{dN}{dt} = 0 \quad \text{or} \quad \dot{N}_1 = -\dot{N}_2$$

$$\frac{dU}{dt} = 0$$

that is, the time variations of the mass of the gas contained in the compressor and of the energy content of this gas are both zero. Also, $\dot{Q} = 0$ since there is no heat transfer to the gas, and $\dot{W} = \dot{W}_s$ since the system boundaries (the compressor) are not changing with time. Thus we have

$$\dot{W}_s = \dot{N}_1 H_2 - \dot{N}_1 H_1 = \dot{N}_1 C_p(T_2 - T_1)$$

or

$$\dot{W}_s = C_p(T_2 - T_1)$$

where $\dot{W}_s = \dot{W}/\dot{N}_1$ is the work done per mole of gas. Therefore, the power necessary to drive the compressor can be computed once the outlet temperature of the gas is known, or the outlet temperature can be determined if the power input is known.

We are at an impasse; we need more information before a solution can be obtained. It is clear by comparison with the previous examples why we cannot obtain a solution here. In the previous cases, the mass balance and the energy balance, together with the equation of state of the fluid and the problem statement provided the information necessary to determine the final state of the system. However, here we have a situation where the energy balance contains two unknowns, the final temperature and $W_s$. Since neither is specified, we need additional information about the system or process before we can solve the problem. This additional information will be obtained in the next chapter.
ILLUSTRATION 3.5-1
Illustration 2.5-4 Continued, Using the Entropy Balance

In Illustration 2.5-4 we attempted to estimate the exit temperature and power requirements for a gas compressor. From the steady-state mass balance we found that

$$ \dot{N}_1 = -\dot{N}_2 = \dot{N} \quad \text{(a)} $$

and from the steady-state energy balance we had

$$ \dot{W}_s = \dot{N} C_p^v(T_2 - T_1) \quad \text{(b)} $$

Now, writing a molar entropy balance for the same system yields

$$ 0 = (S_1 - S_2)\dot{N} + \dot{S}_{\text{gen}} \quad \text{(c)} $$

To obtain an estimate of the exit temperature and the power requirements, we assume that the compressor is well-designed and operates reversibly, that is

$$ \dot{S}_{\text{gen}} = 0 \quad \text{(d)} $$

Thus, we have

$$ S_1 = S_2 \quad \text{(e)} $$

which is the additional relation for a state variable needed to solve the problem. Now using Eq. 3.4-3

$$ S(P_2, T_2) - S(P_1, T_1) = C_p^v \ln \left( \frac{T_2}{T_1} \right) - R \ln \left( \frac{P_2}{P_1} \right) $$

and recognizing that $S(P_2, T_2) = S(P_1, T_1)$ yields

$$ \left( \frac{T_2}{T_1} \right) = \left( \frac{P_2}{P_1} \right)^{\frac{R}{C_p^v}} \quad \text{(f)} $$

or

$$ T_2 = T_1 \left( \frac{P_2}{P_1} \right)^{\frac{R}{C_p^v}} = 290 \text{ K} \left( \frac{10}{1} \right)^{\frac{8.314}{29.3}} = 557.4 \text{ K} \text{ or } 284.2 ^\circ \text{C} \quad \text{(g)} $$

Thus $T_2$ is known, and hence $W_s$ can be computed

$$ W_s = C_p^v(T_2 - T_1) = 29.3 \times (557.4 - 290) = 7834.8 \text{ J/mol} $$

and

$$ \dot{W}_s = \dot{N} W_s = 2.5 \frac{\text{mol}}{\text{s}} \times 7834.8 \frac{\text{J}}{\text{mol}} = 19.59 \frac{\text{kJ}}{\text{s}} $$

Before considering the problem to be solved, we should try to assess the validity of the assumption $\dot{S}_{\text{gen}} = 0$. Unfortunately, this can only be done by experiment. One method is to measure the inlet and exit temperatures and pressures for an adiabatic turbine and see if Eq. e is satisfied. Experiments of this type indicate that Eq. e is reasonably accurate, so that reversible operation is a reasonable approximation for a gas compressor.
Problem 3

Method: UNIQUAC

$P_{\text{eq}} = 0.33 \text{ bar}$

$X_{\text{liq}} \approx 0.21$

$y = 0.3$
Problem 4

propane-butane-flash

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Page 1
propane-butane-flash
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FLASH SEPARATOR EXAMPLE
RUN CONTROL SECTION

RUN CONTROL INFORMATION

THIS COPY OF ASPEN PLUS LICENSED TO SOUTH DAKOTA SCHOOL MINE

TYPE OF RUN: NEW

INPUT FILE NAME: _3447wp1.inm

OUTPUT PROBLEM DATA FILE NAME: _3447wp1

LOCATED IN:

PDF SIZE USED FOR INPUT TRANSLATION:
NUMBER OF FILE RECORDS (PSIZE) = 0
NUMBER OF IN-CORE RECORDS = 256
PSIZE NEEDED FOR SIMULATION = 256

CALLING PROGRAM NAME: apmain
LOCATED IN: C:\PROGRA~1\ASPENT~1\ASPENP~2.5\Engine\xeq

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

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FLASH SEPARATOR EXAMPLE
Page 2
propane-butane-flash

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

<table>
<thead>
<tr>
<th>STREAM</th>
<th>SOURCE</th>
<th>DEST</th>
<th>STREAM</th>
<th>SOURCE</th>
<th>DEST</th>
</tr>
</thead>
<tbody>
<tr>
<td>FEED</td>
<td>----</td>
<td>FLASH</td>
<td>VAPOR</td>
<td>FLASH</td>
<td>----</td>
</tr>
<tr>
<td>LIQUID</td>
<td>FLASH</td>
<td>----</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

FLOWSHEET CONNECTIVITY BY BLOCKS

<table>
<thead>
<tr>
<th>BLOCK</th>
<th>INLETS</th>
<th>OUTLETS</th>
</tr>
</thead>
<tbody>
<tr>
<td>FLASH</td>
<td>FEED</td>
<td>VAPOR LIQUID</td>
</tr>
</tbody>
</table>

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:
S-1 FLASH
(RETURN S-1)

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CONVENTIONAL COMPONENTS (KMOL/HR)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PROPANE</td>
<td>0.500000</td>
<td>0.500000</td>
</tr>
<tr>
<td>BUTANE</td>
<td>0.500000</td>
<td>0.500000</td>
</tr>
<tr>
<td>TOTAL BALANCE</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MOLE(KMOL/HR )</td>
<td>1.00000</td>
<td>1.00000</td>
</tr>
<tr>
<td>MASS(KG/HR )</td>
<td>51.1100</td>
<td>51.1100</td>
</tr>
<tr>
<td>ENTHALPY(CAL/SEC )</td>
<td>-8766.05</td>
<td>-8223.13</td>
</tr>
</tbody>
</table>

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FLASH SEPARATOR EXAMPLE
SENSITIVITY BLOCK SECTION

SENSITIVE BLOCK: 5-1

SAMPLED VARIABLES:
VAPFLO : TOTAL MOLEFLOW IN STREAM VAPOR SUBSTREAM MIXED

VARIED VARIABLES:
VARY 1: SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK FLASH
LOWER LIMIT = 1.0000 ATM
UPPER LIMIT = 10.0000 ATM
INCREMENT = 0.5000

TABULATED VARIABLES:
COLUMN 2: VAPFLO

<table>
<thead>
<tr>
<th>VARY 1</th>
<th>VAPFLO</th>
</tr>
</thead>
<tbody>
<tr>
<td>FLASH</td>
<td></td>
</tr>
<tr>
<td>PARAM</td>
<td></td>
</tr>
<tr>
<td>PRES</td>
<td></td>
</tr>
<tr>
<td>ATM</td>
<td>KMOL/HR</td>
</tr>
<tr>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>
propane-butane-flash

| ! | 1.5000 ! 1.0000 ! 
| ! | 2.0000 ! 1.0000 ! 
| ! | 2.5000 ! 1.0000 ! 
| | 3.0000 | 1.0000 |
|-----|------------------|
| ! | 3.5000 ! 1.0000 ! 
| ! | 4.0000 ! 1.0000 ! 
| ! | 4.5000 ! 1.0000 ! 
| ! | 5.0000 ! 1.0000 ! 
| ! | 5.5000 ! 1.0000 ! 
| ! | 6.0000 ! 0.9922 ! 
| ! | 6.5000 ! 0.7459 ! 
| ! | 7.0000 ! 0.5369 ! 
| ! | 7.5000 ! 0.3417 ! 
| ! | 8.0000 ! 0.1453 ! 
| ! | 8.5000 ! 0.0 ! 
| ! | 9.0000 ! 0.0 ! 
| ! | 9.5000 ! 0.0 ! 
| ! | 10.0000 ! 0.0 ! 
| ! | 7.1000 ! 0.4973 ! 

\[ VAPFLO = 0.497287 \text{ \text{KMOL/HR}} \]

**COMPONENTS**

<table>
<thead>
<tr>
<th>ID</th>
<th>TYPE</th>
<th>FORMULA</th>
<th>NAME OR ALIAS</th>
<th>REPORT NAME</th>
</tr>
</thead>
<tbody>
<tr>
<td>PROPANE</td>
<td>C</td>
<td>C3H8</td>
<td>C3H8</td>
<td>PROPANE</td>
</tr>
<tr>
<td>BUTANE</td>
<td>C</td>
<td>C4H10-1</td>
<td>C4H10-1</td>
<td>BUTANE</td>
</tr>
</tbody>
</table>

**BLOCK: FLASH MODEL: FLASH2**

- INLET STREAM: FEED
- OUTLET VAPOR STREAM: VAPOR
- OUTLET LIQUID STREAM: LIQUID
- PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th>TOTAL BALANCE</th>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE(KMOL/HR)</td>
<td>1.0000</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>MASS(KG/HR)</td>
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<td>51.1100</td>
<td>0.129291E-12</td>
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<tr>
<td>ENTHALPY(CAL/SEC)</td>
<td>-8766.05</td>
<td>-8223.13</td>
<td>-0.619342E-01</td>
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</tbody>
</table>

**INPUT DATA**

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---

Method chosen
propane-butane-flash

SPECIFIED TEMPERATURE K 313.150
SPECIFIED PRESSURE ATM 7.10000
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

*** RESULTS ***

OUTLET TEMPERATURE K 313.15
OUTLET PRESSURE ATM 7.1000
HEAT DUTY CAL/SEC 542.92
VAPOR FRACTION 0.49729

V-L PHASE EQUILIBRIUM :

<table>
<thead>
<tr>
<th>COMP</th>
<th>F(I)</th>
<th>X(I)</th>
<th>Y(I)</th>
<th>K(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PROPANE</td>
<td>0.50000</td>
<td>0.36888</td>
<td>0.63255</td>
<td>1.7148</td>
</tr>
<tr>
<td>BUTANE</td>
<td>0.50000</td>
<td>0.63112</td>
<td>0.36745</td>
<td>0.58223</td>
</tr>
</tbody>
</table>

ASPEN PLUS PLAT: WIN32 VER: 21.0
FLASH SEPARATOR EXAMPLE
STREAM SECTION

FEED LIQUID VAPOR
-------------------
STREAM ID FEED LIQUID VAPOR
FROM: ---- FLASH FLASH
TO: FLASH ---- ----

SUBSTREAM: MIXED
PHASE: LIQUID LIQUID VAPOR
COMPONENTS: KMOL/HR
PROPANE 0.50000 0.1854 0.3146
BUTANE 0.50000 0.3173 0.1827
COMPONENTS: MOLE FRAC
PROPANE 0.50000 0.3689 0.6325
BUTANE 0.50000 0.6311 0.3675

TOTAL FLOW:
KMOL/HR 1.0000 0.5027 0.4973
KG/HR 51.1100 26.6182 24.4917
L/MIN 1.6444 0.8390 25.8055

STATE VARIABLES:
TEMP K 313.1500 313.1500 313.1500
PRES ATM 10.0000 7.1000 7.1000
VFRAC 0.0 0.0 1.0000
LFRAC 1.0000 1.0000 0.0
SFRACT 0.0 0.0 0.0

ENTHALPY:
CAL/MOL -3.1558+04 -3.2381+04 -2.6795+04
CAL/GM -617.4484 -611.5545 -544.0514
CAL/SEC -8766.0457 -4521.8027 -3701.3245

ENTROPY:
CAL/MOL-K -90.9658 -94.2574 -74.9056
CAL/GM-K -1.7798 -1.7802 -1.5209

DENSITY:
MOL/CC 1.0135-02 9.9862-03 3.2118-04
GM/CC 0.5180 0.5288 1.5818-02
AVG MW 51.1100 52.9491 49.2507

ASPEN PLUS PLAT: WIN32 VER: 21.0
FLASH SEPARATOR EXAMPLE
PROBLEM STATUS SECTION

BLOCK STATUS

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propane-butane-flash

* Calculations were completed normally
* All Unit Operation blocks were completed normally
* All streams were flashed normally
* All Sensitivity blocks were completed normally

* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
### PROPANE-BUTANE FLASH - Vapor Outlet conditions

<table>
<thead>
<tr>
<th>P (ATM)</th>
<th>T (K)</th>
<th>DENSITY (MOL/CC)</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.1</td>
<td>313.15</td>
<td>3.21E-04</td>
<td>0.86</td>
</tr>
</tbody>
</table>

\[
Z = \frac{P}{\rho RT}
\]

\[Z \neq 1.0\]

Vapor phase is non-ideal.

Reyn-Robinson EOS better than "Ideal" method.