COMPUTATIONAL THERMODYNAMICS AND HEAT TRANSFER DEVICES

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INTRODUCTION

AIM OF THE PROJECT :

- Learning the basic concepts of Thermodynamics and Heat Transfer Device
- Computation of various thermodynamic properties
- Application of heat transfer devices to evaluate its temperature distribution
- Implementation of Finite Difference Method and Discretization Techniques for PDE Toolbox in MATLAB

THERMODYNAMICS

This study is done majorly as there is a need to relate work produced and heat supplied. Then emerged the three important governing laws, the laws of thermodynamics. These laws find application in all branches of science and engineering which includes the calculation of heat and work requirements for various processes.Thus the the study and application of thermodynamics is very crucial.

HEAT TRANSFER

Heat energy exists in various forms. Heat is the form of energy that can be transferred from one system to another as a result of temperature difference. The science that deals with the determination of the rates of such energy transfers is heat transfer

LECTURE 1 Volumetric Properties of Fluid

- PVT Behaviour of Pure Substances
- PV Diagram and Critical Behaviour
- Single Phase Regions
- Virial Equation of State
- Cubic Equations of State
- Generic Cubic Equations of State
- Parameters for EOS

LECTURE 2 LECTURE 3

● Residual properties and its derivations

Gibbs residual function

● Enthalpy and entropy departure functions

● Residual properties from the virial equation of states

- Finding molar volume using departure function
- PV curve for SRK equation of state

LECTURE 4 LECTURE 5 LECTURE 6

- Chemical potential and Equilibrium
- Partial properties
- Partial properties for binary solution
- The ideal gas state mixture model

- Fugacity of pure species
- Excess property and activity coefficient
- Gamma- Phi formulation of VLE
- Correlations for liquid phase activity
- Van-Laar Equation
- Local-Composition Model

- Heat transfer Mechanisms
- Conduction
- Convection
- **Radiation**

LECTURE 7 LECTURE 8 LECTURE 9

- Introduction to heat transfer
- Heat conduction equation
- Numerical methods in heat conduction
- 2D transient heat conduction equation

- Fundamentals of convection
- Physical mechanism
- Classification of fluid flow
- Boundary layer

- Heat exchangers
- Its types
- The overall heat transfer coefficient
- Fouling factor
- LMTD Method
- Multipass and Cross-Flow Heat Exchangers

Volumetric properties of fluid

THE PHASE RULE

The number of independent variables that must be fixed to egt the intensive state with respect to the multiphase system in equilibrium is called the degree of freedom of the system. $|F = 2 - \pi + N|$ *(Gibbs phase rule)*

SINGLE PHASE REGIONS

The unique relation connecting P,V, and T and which can be expressed analytically as $f(P,V,T)=0$. This relation is known as PVT equation of state. It relates pressure, molar or specific volume, and temperature for a pure homogeneous fluid at equilibrium.

Volume expansivity: $\beta = 1/V(\partial V/\partial T)P$. Isothermal compressibility: $κ = -1/V(∂V/∂P)$ ^T

IDEAL GAS AND IDEAL-GAS STATE

The equation of state describes PVT behaviour of gases for many practical purposes near ambient conditions of T and P. This equation of state is therefore understood to define an ideal gas and to represent a model of behavior more or less approximating the behavior of real gases. It is called the ideal gas law, but is in fact valid only for pressures approaching zero and temperatures approaching infinity.

A GENERIC CUBIC EQUATION OF STATE

Z = β + (Z + εβ)(Z + σβ) (1 + β − Z)/(qβ) β = ΩP/r Trq = Ψα(Tr; ω)/ΩTr

 $P = RT/(V - b) - a(T)/(V + εb)(V + σb)$ β ≡ bP/ RT q ≡ a(T)/bRT $Z = 1 + β - qβ (Z - β)/(Z + εβ)(Z + σβ)$

THERMODYNAMIC PR0PERTIES OF FLUIDS

RESIDUAL PROPERTIES

Residual property is the difference between actual and ideal gas state values at same temperature and pressure.the residual volume for example is $Vr \equiv V - Vig = V - RT/P$ because $V = ZRT/P$.

Therefore the generic residual property is defined by $\sqrt{MR} = M - Mig$ where M, Mig are actual and ideal gas state properties at same temperature. From a practical perspective this equation divides property calculations into two parts: first, simple calculations for properties in the ideal-gas state; second, calculations for the residual properties, which have the nature of corrections to the ideal-gas-state values.

RESIDUAL PROPERTIES FROM THE VIRIAL EQUATIONS OF STATE

The numerical or graphical evaluation of integrals is often tedious and imprecise. An attractive alternative is analytical evaluation through equations of state. The procedure depends on whether the equation of state is volume explicit, i.e., expresses V (or Z) as a function of P at constant T, or pressure explicit, i.e., expresses P (or Z) as a function of V (or ρ) at constant T.

Volume Explicit $Z - 1 = BP/RT$. GR $/RT = BP/RT$ HR $/RT = P/R$ (B $T - dB/dT$) SR $/R = -PdB/RdT$

Pressure-explicit three-term virial equation: $Z - 1 = B\rho + C\rho 2$

PROBLEM STATEMENT 1

AIM : To calculate the molar volumes of saturated vapor and saturated liquid n-butane, n-pentane, n-hexane, n-heptane using cubic equations of state and plot the separate graphs of molar volume of saturated vapor v/s acentric factor (w) for SRK and PR equations of state.

GIVEN : Critical point information of different compounds

APPROACH :

The values of z for different fluid exhibit similar behaviour when correlated as a function of reduced temperature and reduced pressure.

Tr=T/Tc ; Pr=P/Pc; β=ΩPr/Tr; q= ψ∝(Tr;ω)/ΩTr;

 $Z=z\Delta$ 3 + $z\Delta$ ($\varepsilon\beta$ + $\sigma\beta$ - 1 - β) + $z(q\beta - (1 + \beta)(\sigma + \varepsilon)\beta + \sigma\varepsilon\beta\Delta2)$ - ($\sigma\varepsilon\beta\Delta2$ + $\sigma\epsilon\beta\Delta3$ + $q\beta\Delta2$)

Roots of these equations are found and we get 3 roots. We assign the smallest root to the compressibility factor of the liquid and the largest root to the compressibility factor of the vapour. Then molar volume can be calculated by putting the value of z in the following equation, $V=ZRT/P$.

Parameters assignments for equations of state

 α SRK(Tr; ω) = [1 + (0.480 + 1.574 ω − 0.176 ω^2)(1 − Tr ^(1/2))] ^2 α PR(Tr; ω) = [1 + (0.37464 + 1.54226 ω − 0.26992 ω^2)(1 − Tr ^(1/2))] ^2

Matlab code

For Vdw

```
disp('Q1= finding molar volumes, Q2= graphs')
Q = input('question no.=');disp('5) vdw, 6) RK, 7) SRK, 8) PR');
m=input('choose method:');
if 0 == 1disp('1)n-butane, 2)n-pentane, 3)n-hexane, 4)n-heptane');
c=input('choose compound:');
T = input('temperature:');P = input('pressure:');T c= input('critical temperature:');
P c= input('critical pressure:');
P r = P/P C;
T = T/T c;R = 83.14;w=0:
if c == 1 w = 0.199; end
if c == 2 w = 0.251; end
if c == 3 w = 0.299; end
if c==4 w=0.349; end
```
 $if m==5$ $a=1$: $s=0$: $e=0$: $o=1/8$: $p=27/64;$ $B = (o*P r)/T r;$ $q = (p * a) / (o * T r)$; $q=e*B+s*B-1-B;$ $h = ((q * B) - ((1+B) * (s+e) * B) + (s * e * B * B))$; $l=-s*e*B*B-s*e*B*B*B-q*B*B;$ $z = [1 q h 1];$ $r = roots(z)$; fprintf(' $\frac{3.4f}{n}$, r); $r1 = max(r)$; $r2 = min(r);$ $Vv = (r1*R*T)/P$; $V = (r2*R*T)/P$ fprintf('\nmolar volume of saturated vapour=%.4f cm^3/mol\n', Vv); fprintf('\nmolar volume of saturated liquid=%.4f cm^3/mol\n',Vl); end

Graphs of molar volume of saturated vapor v/s acentric factor

1) SRK 2) PR

From the above graph we can say that molar volume of saturated vapour is increasing rapidly with the increase in acentric factor

PROBLEM STATEMENT 2

Given: Equation of state and critical point information

Aim : To obtain PV diagram for the system

Equation of state : PR ; System: Ammonia ;

Critical point information : Pc- 11280 kPa Tc - 405.65 K w- 0.2526

MATLAB CODE

 $P C=112.8;$ $T_c = 405.65;$ $w = 0.2526;$ $P = 0$; $T=0$; $V=0$; % cubic equation of state

 $R = 83.14;$

 \equiv

 $b = (0.07780*R*T_c)/P_c;$

axis([0 1000 -500 500]); xlabel('Volume in cm3/mol') ylabel ('pressure in bar') title('PV diagram')

OBSERVATIONS

• For temperature greater than critical temperature, pressure decreases with increase in the volume. • For temperatures less than critical temperature, pressure first decreases rapidly with increase in volume then after a certain point it increases and reaches a maximum and then decreases again.

 • At critical temperature there is an inflection in the graph.

• In the vapor region, above critical temperature, pressure decreases with increase in volume, below critical temperature, with increase in volume it decreases rapidly in the liquid region. It then reaches minimum and then rise and reach maximum and then decrease again in the liquid vapour saturated region.

• Thus with just critical point information and equation of state one can plot PV diagram without the use of Antoine equation

THE FRAMEWORK OF SOLUTION THERMODYNAMICS

THE CHEMICAL POTENTIAL AND EQUILIBRIUM

 $\sum \mu_i dn_i = 0$

The equation represents a general criterion for chemical reaction equilibrium in a single phase closed PVT system, and is basis for the development of the working equations for the solution of reaction-equilibrium problems.

Multiple phases at the same T and P are in equilibrium when the chemical potential of each species is the same in all phases

μi $\alpha = \mu i \beta = -\mu i \pi$ (i = 1, 2, ..., N)

PARTIAL PROPERTIES

It is a measure of the response of total property nM to the addition of an infinitesimal amount of

species i to a finite amount of solution, at constant T and P.

∂ (nM $\overline{M}_i \equiv$

GIBBS/DUHEM

$$
\sum_{i} x_{i} d\overline{M}_{i} = \left(\frac{\partial M}{\partial P}\right)_{T, x} dP + \left(\frac{\partial M}{\partial T}\right)_{P, x} dT
$$

PARTIAL PROPERTIES FOR BINARY SOLUTION

For binary systems

 $M = x_1 \overline{M}_1 + x_2 \overline{M}_2$

 $dM = x_1 d\bar{M}_1 + \bar{M}_1 dx_1 + x_2 d\bar{M}_2 + \bar{M}_2 dx_2$

When M is known as a function of x1 at constant T and P, the appropriate form of the Gibbs/ Duhem equation is $x_1 dM_1 + x_2 dM_2 = 0$

THE IDEAL-GAS-STATE MIXTURE MODEL

The ideal-gas-state mixture model provides a conceptual basis upon which to build the structure of solution thermodynamics. It is a useful property model because it: has a molecular basis,approximates reality in the well-defined limit of zero pressure, is analytically simple.

A partial molar property (other than volume) of a constituent species in an ideal-gas-state mixture is equal to the corresponding molar property of the species in the pure ideal-gas state at the mixture temperature but at a pressure equal to its partial pressure in the mixture. This is expressed mathematically for generic partial property M^{$-$} i ig \neq V $-$ i ig by the equation:

$$
\bar{M}_i^{ig}(T,P) = M_i^{ig}(T,p_i)
$$

FUGACITY OF PURE SPECIES

Vapor/Liquid Equilibrium for Pure Species

For a pure species, coexisting liquid and vapor phases are in equilibrium when they have the same temperature, pressure, and fugacity $f_i^v = f_i^l = f_i^{\text{sat}}$

Fugacity of a Pure Liquid

$$
f_i^l(P) = \frac{f_i^v(P_i^{\text{sat}})}{P_i^{\text{sat}}} \frac{f_i^l(P_i^{\text{sat}})}{f_i^v(P_i^{\text{sat}})} \frac{f_i^l(P)}{f_i^l(P_i^{\text{sat}})} P_i^{\text{sat}}
$$

$$
f_i = \phi_i^{\text{sat}} P_i^{\text{sat}} \exp\left(\frac{1}{RT} \int_{P_i^{\text{sat}}}^P V_i^l dP\right)
$$

Because Vi l , the liquid-phase molar volume, is a very weak function of P at temperatures well below Tc, an excellent approximation is often obtained by taking Vi l to be constant at the value for saturated liquid. In this case,

$$
f_i = \phi_i^{\text{sat}} P_i^{\text{sat}} \exp \frac{V_i^l (P - P_i^{\text{sat}})}{RT}
$$

THERMODYNAMIC FORMULATIONS FOR VAPOUR/LIQUID EQUILIBRIUM

EXCESS GIBBS ENERGY AND ACTIVITY COEFFICIENTS

$$
\bar{G}_i - \bar{G}_i^{id} = RT \ln \frac{f_i}{x_i f_i}
$$

Left side of this equation is the partial excess Gibbs energy G $^-$ i E; the dimensionless ratio f $\hat{ }$ i⁄xi fi appearing on the right is the activity coefficient of species i in solution, symbol γi. Thus, by definition

$$
\gamma_i \equiv \frac{\hat{f}_i}{x_i f_i}
$$

$$
\bar{G}_i^E = RT \ln \gamma_i
$$

THE GAMMA/PHI FORMULATION OF VLE

for species in the liquid phase $\hat{f}_i^l = x_i \gamma_i^l f$

$$
V_i^l \qquad \boxed{y_i \Phi_i P = x_i \gamma_i P_i^{\text{sat}} \qquad (i = 1, 2, \dots, N)} \quad \Phi_i \equiv \frac{\hat{\phi}_i^{\nu}}{\phi_i^{\text{sat}}} \exp \left[-\frac{V_i^l (P - P_i^{\text{sat}})}{RT}\right]
$$

The vapor pressure of pure species i is most commonly

given by the Antoine equation:

$$
n P_i^{\text{sat}} = A_i - \frac{B_i}{T + C_i}
$$

CORRELATIONS FOR LIQUID-PHASE ACTIVITY COEFFICIENTS

GE∕RT is a function of T, P, and composition, but for liquids at low to moderate pressures it is a very weak function of P. Therefore its pressure dependence is usually neglected, and for applications at constant T, excess Gibbs energy is treated as a function of composition alone

$$
\frac{G^E}{RT} = g(x_1, x_2, \ldots, x_n)
$$

The Redlich/Kister Expansion

$$
G \equiv G^{E}/(x_{1}x_{2}RT), \qquad \qquad \ln \gamma_{1} = x_{2}^{2}\left(Y + x_{1}\frac{dY}{dx_{1}}\right) \qquad \qquad \ln \gamma_{2} = x_{1}^{2}\left(Y - x_{2}\frac{dY}{dx_{1}}\right)
$$

Margules equations

$$
\frac{G^E}{RT} = (A_{21}x_1 + A_{12}x_2)x_1x_2
$$
\n
$$
\boxed{\ln \gamma_1 = x_2^2 [A_{12} + 2(A_{21} - A_{12})x_1]}
$$
\n
$$
\boxed{\ln \gamma_2 = x_1^2 [A_{21} + 2(A_{12} - A_{21})x_2]}
$$

 (For the limiting conditions of infinite dilution,) $\ln \gamma_1^{\infty} = A_{12}$ and $\ln \gamma_2^{\infty} = A_{21}$

The van Laar Equation

$$
\ln \gamma_1 = A'_{12} \left(1 + \frac{A'_{12} x_1}{A'_{21} x_2} \right)^{-2} \qquad \ln \gamma_2 = A'_{21} \left(1 + \frac{A'_{21} x_2}{A'_{12} x_1} \right)^{-2}
$$

PROBLEM STATEMENT 3

Vapor-Liquid Equilibrium curves

SYSTEM :

System-1: Ethanol & Water

Wilson's Equation

MODEL:

$$
\ln \gamma_1 = -\ln(x_1 + \Lambda_{12}x_2) + x_2 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{x_2 + \Lambda_{21}x_1} \right]
$$

\n
$$
\ln \gamma_2 = -\ln(x_2 + \Lambda_{21}x_1) - x_1 \left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{x_2 + \Lambda_{21}x_1} \right]
$$

\n
$$
A_{12} = \lambda_{12} - \lambda_{11}
$$

\nWhere,
\n
$$
A_{21} = \lambda_{21} - \lambda_{22}
$$

\n
$$
\Delta_{ij} = \frac{V_j}{V_i} \exp \left[-\frac{(\lambda_{ij} - \lambda_{ii})}{RT} \right]
$$

CODE

```
A 12 = -75.8523;
 A 21 = 1058.3059; V1 = 58.69; \text{m1/mol}V2 = 18.07; m1/molR = 1.98; P=90;plsat=90; p2sat = 90;x=0:0.1:1:t0 =zeros(1, 11);
 y1=0; y2=0;tlsat=(B1/(A1-log10(P)))-C1; t2sat=(B2/(A2-log10(P)))-C2;
 T = 300;
 A1= 8.11220 ; A2= 8.07131 ; %Antoine's constants
 B1 = 1592.864; B2 = 1730.630;
 C1 = 226.184; C2 = 233.426;
 fprintf('x1 y1\n');
\exists for i= 1:20
     T = (t1sat.*x(i)+t2sat.*(1-x(i)))+273.15;L12 = (V2/V1) * exp(-A 12/(R*T));L21 = (V1/V2) * exp(-A 21/(R*T));q1 = exp(-log(x(i) + (1-x(i)) \cdot *L12) + ((1-x(i)) \cdot *((L12 \cdot (x(i) + (1-x(i)) \cdot *L12)) - (L21 \cdot ((1-x(i)) + x(i) \cdot *L21))))q2 = exp(-log((1-x(i)) + x(i), xL21)) - (x(i), x((L12.7(x(i)+(1-x(i)), xL12)) - (L21.7((1-x(i))+x(i), xL21))))plsat = 10^{(A1-(B1/((T-273)+C1))});
     p2sat = 10^{(A2-(B2/((T-273)+C2))});
      y1 = (x(i) * q1 * p1sat) / (P);
     y2 = ((1-x(i)) * q2 * p2sat) / (P);t0=T;
 end
 plot(x, y1);
```
HEAT TRANSFER

A thermodynamic analysis is concerned with the amount of heat transfer as a system undergoes a process from one equilibrium state to another. The science that deals with the determination of the rates of such energy transfers is the heat transfer

Heat can be transferred in three different modes: conduction, convection, and radiation.

HEAT EXCHANGERS

Heat exchangers are devices that facilitate the exchange of heat between two fluids that are at different temperatures while keeping them from mixing with each other. Heat transfer in a heat exchanger usually involves convection in each fluid and conduction through the wall separating the two fluids.

In the analysis of heat exchangers, it is convenient to work with an overall heat transfer coefficient U or a total $\frac{1}{UA_{c}} = \frac{1}{U.A_{c}} = \frac{1}{U.A_{c}} = R = \frac{1}{h.A_{c}} + R_{wall} + \frac{1}{h.A_{c}}$ thermal resistance R, expressed as

In a well-insulated heat exchanger, the rate of heat transfer from the hot fluid is equal to the rate of heat transfer to the cold one

$$
Q = \dot{m}_c c_{pc} (T_{c, \text{ out}} - T_{c, \text{ in}}) = C_c (T_{c, \text{ out}} - T_{c, \text{ in}})
$$

$$
\dot{Q} = \dot{m}_h c_{ph} (T_{h, \text{ in}} - T_{h, \text{ out}}) = C_h (T_{h, \text{ in}} - T_{h, \text{ out}})
$$

PROBLEM STATEMENT 4

ETHANOL :

Ethanol is classified by the National Fire Protection Association (NFPA) as a flammable fluid because of its low flash point of 17 degree C. This means that at 17 degree C or higher, ethanol can vaporize and become a mixture in air that would ignite when an ignition source is present. Thus, in an environment that ignition sources are present, keeping ethanol at a temperature below its flash point can help to prevent fire hazard

GIVEN :

A process where ethanol is cooled by water in a 1-shell-pass heat exchanger that can accommodate a maximum of 14-tube-passes. The tubes are made of copper and thin-walled with an inner diameter of 1.5 cm. The length of each tube pass that can be fitted inside the heat exchanger is 3 m, and the overall heat transfer coefficient is 700 W/m2∙K. Ethanol (cp = 2630 J/kg∙K) enters the heat exchanger at 55°C and flows through the shell at a rate of 0.28 kg/s. Water enters the heat exchanger at 28C and flows through the tubes at a rate of 1.3 kg/s. To prevent fire hazard, the ethanol is to be cooled to 15°C, which is below its flash point.

TO FIND

The number of tube passes that is necessary inside the shell-and tube heat exchanger to cool the ethanol to the prescribed temperature. Discuss whether or not this heat exchanger is suitable for this application. Evaluate any required property of water at 5 degree C. Is this a good assumption? Vary the outlet hot fluid temperature (Th,out) and plot number of tube passes 'n' vs outlet hot fluid temperature (Th,out).

 \cdot The number of tube passes = 12

• The maximum number of tube passes which the heat exchanger can accommodate is 14. Since 12 (12<14) tube passes are sufficient for reducing ethanol temperature from 55 to 15 degree C, this heat exchanger is suitable for this application.

• Tc in for water = 2 degree C ; Tc out = Q/Cc + Tc in = 29456 /5466.5 + 2 = 7.4 degree C therefore , T mean = (Tc in + Tc out)/2 = $(2+7.4)/2 = 4.7 \sim 5$ degree C Hence it is a good assumption

PLOT n vs Thout

PART B

Now, keeping all the inlet conditions (Tc,in and Th,in) to be same, vary the number of tube passes (n) from 1 to 14 and find out the effectiveness and outlet coolant and outlet hot fluid temperatures (Tc,out and Th,out).

n=1 Thout=48.394734 Tcout=2.889805 n=2 Thout=42.710704 Tcout=3.655509 n=3 Thout=37.809886 Tcout=4.315705 n=4 Thout=33.577258 Tcout=4.885888 n=5 Thout=29.916410 Tcout=5.379046 n=6 Thout=26.746127 Tcout=5.806119 n=7 Thout=23.997688 Tcout=6.176366 n=8 Thout=21.612717 Tcout=6.497648 n=9 Thout=19.541455 Tcout=6.776671 n=10 Thout=17.741362 Tcout=7.019164 n=11 Thout=16.175972 Tcout=7.230040 n=12 Thout=14.813952 Tcout=7.413520 n=13 Thout=13.628329 Tcout=7.573237 n=14 Thout=12.595838 Tcout=7.712325

a) Double-pipe: Parallel-flow

b) Double-pipe: Counter-flow

c) Cross-flow (single pass): Cmax mixed, Cmin unmixed

d) Cross-flow (single pass): Cmin mixed, Cmax unmixed

Determine the effectiveness of each of the above mentioned heat exchangers.

% Double-pipe: Parallel-flow = eff1 $eff1=(1-exp((-1)*NTU*(1+c)))/(1+c);$

```
%Double-pipe: Counter-flow = eff2
eff2 = (1-exp((-1) * NTU* (1-c)) ) / (1-c*exp((-1) * NTU* (1-c)) );
```

```
%Cross-flow (single pass): Cmax mixed, Cmin unmixed = eff3
eff3 = (1/c)*(1-exp(-c*(1-exp((-1)*NTU))));
```

```
%Cross-flow (single pass): Cmin mixed, Cmax unmixed = eff4
eff4 = 1-exp(- (1/c) * (1-exp((-c) * NTU)));
```

```
% shell tube
eff5=2*(1+c+((1+c^2)*(1/2)). * (1+exp((-1)*NTU.*(1+c^2)^(1/2))). / (1-exp((-1)*NTU.*(1+c^2)^(1/2)))))^(-1)
```


Application of different types of heat exchangers are as follows:

Double pipe heat exchangers

- Chemical industries
- Food processing industries
- Oil and gas industries

Shell and tube heat exchangers

- Refrigeration
- Pharmaceuticals
- Power generation

Cross flow heat exchangers

- Cooling industries
- Automobile radiators
- Condenser in steam system

We can see that the shell and tube type of heat exchanger is used in our daily life, because of its us in refrigeration

THANK YOU