

CODATHON

(Final Round)

Name:

Time: 3 hrs

- 1) Vapour-liquid equilibrium (VLE) is a very important subject to be studied by chemical engineers. It is the most important concept to be able to design distillation columns (which contribute to roughly 95% of all separation processes used in the industry) and flash evaporators. For those who are unaware of what vapour-liquid equilibrium is, a brief explanation is given as follows:

Consider a closed container just having water. Some water molecules on the surface evaporate and form the vapour phase and occupy the empty space in the closed vessel. The pressure exerted by this vapour (empty space is known as head space in a container) in the head space is termed as vapour pressure. Simultaneously, some water molecules from the vapour phase condense and become a part of the liquid phase. A point is reached when the rate of evaporation becomes equal to the rate of condensation and there is no further change in the amounts of liquid and vapour phases and hence no further change in the vapour pressure. This can be understood as vapour-liquid equilibrium. So, at any given temperature, the vapour pressure of the vapours in the head space in equilibrium with liquid can be found using the Antoine equation which is given as follows:

$$\ln V_p = A - \frac{B}{(T + C)}$$

The constants A, B and C are dependent on the material. Thus one can find out the amount of vapours in the head space in equilibrium with a given liquid phase at a given temperature. This is very important when flammable liquids are stored in closed vessels and one must ensure that an explosive or flammable mixture is not being formed in the vapor head space. A liquid is said to boil when its vapour pressure at a given temperature becomes equal to the atmospheric pressure. Thus for water, the boiling point is 100°C at sea level. This is why, when you go to hill stations, water boils at a lower temperature as the atmospheric pressure is lower there.

Now that you have some idea about VLE, let us extend this to multicomponent mixtures as this is what we deal in most cases. Instead of just water, you may now imagine a mixture of water and acetic acid. Now, we would have to be concerned about what is the composition of the mixture in the liquid phase and what is the composition of the vapour phase that is in equilibrium with this liquid. In VLE, almost always we define composition of the liquid and vapour phases in mole fractions. Given a liquid mixture having certain composition, the bubble point temperature is the temperature at which the first bubble is formed or you can think of it as the “boiling point” for the liquid mixture that you have. Given a vapour mixture having certain composition, the dew point temperature is the temperature at which the first drop of liquid is formed by condensation and can be thought of as the “condensation temperature” of the vapour mixture. Water boils at 100°C and acetic acid boils at roughly 118°C, however a liquid mixture of these two will boil at some temperature between 100 and 118°C depending on the composition of the liquid mixture.

One of the easiest ways to perform VLE calculations is by the use of Raoult’s law for ideal solutions. Consider a closed container at some temperature T and pressure P. Let us say that the container contains a multicomponent mixture and the vapour and liquid phases are in equilibrium with each other. Let x_i denote the mole fraction of the i^{th} component in the liquid phase and y_i be the vapour phase mole fraction of the i^{th} component. By Raoult’s law,

$$Py_i = x_i P_i^{sat}$$

where P_i^{sat} is the vapor pressure of pure component i at temperature T. Writing these equations for each and every component and solving them, you can determine the bubble point temperature, vapour composition in equilibrium with a given liquid composition, etc.

- A) Consider an ideal four-component mixture (Raoult's law is applicable) having 10% ethylene, 25% ethane, 50% propane and rest n-butane (all these are mole percents). The Antoine equation constants are given in the table below. Calculate the bubble point and dew point temperatures of this mixture at pressures of 16, 18 and 20 atm. Note that 1atm= 760 mm Hg

Compound	A	B	C
Ethylene	6.6438	395.74	266.681
Ethane	6.82915	663.72	256.681
Propane	6.80338	804	247.04
n-Butane	6.80776	935.77	238.789

In the Antoine equation given here, vapour pressure is expressed in mm Hg and temperature is in °C.

These calculations become important for a chemical engineer in cases such as transportation of LPG. One must take care that liquid streams being transported don't vapourize due to presence of valves that may reduce the pressure and thereby the temperature. **[10 marks]**

Now that you have an idea of VLE calculations, let us make stuff more realistic. The Raoult's law is a very idealised relation that works well only for a few mixtures at certain conditions. A first step in creating a more accurate estimate is adding sort of a correction factor termed as the activity coefficient. The Raoult's law can be modified as follows:

$$Py_i = x_i \gamma_i P_i^{sat}$$

where γ_i is the activity coefficient of the i^{th} component and this is a function of the liquid phase compositions and the temperature.

- B) For a methanol (1) / methyl acetate (2) binary system, reasonable correlations for the activity coefficients are given by

$$\ln \gamma_1 = Ax_2^2, \quad \ln \gamma_2 = Ax_1^2 \quad \text{and} \quad A = 2.771 - 0.00523T \quad (\text{T is in K})$$

The Antoine equation provides expressions for vapour pressures (kPa) :

$$\ln P_1^{sat} = 16.59158 - \frac{3643.31}{(T-33.324)} \quad , \quad \ln P_2^{sat} = 14.25326 - \frac{2665.54}{(T-53.424)}$$

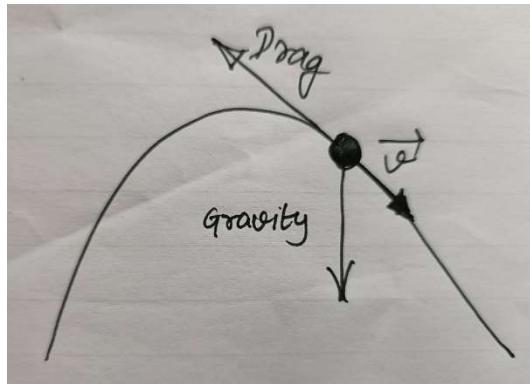
where T is temperature in K

Estimate:

- P and y_1 for $T=318.15$ K and $x_1=0.25$
- P and x_1 for $T=318.15$ K and $y_1=0.60$
- T and y_1 for $P=101.33$ kPa and $x_1=0.85$
- T and x_1 for $P=101.33$ kPa and $y_1=0.40$

[10 marks]

- 2) Projectile motion is something all of us have learnt in our college physics course. Since we were mere college students, we were engaged in the study of projectile motions with a simple parabolic profile. Now that you know coding, let us now solve projectile motion from a more realistic approach and let us include the drag force exerted on the object by air.



The drag force acts in the direction opposite to the velocity vector and has a magnitude proportional to v^2 . Let \hat{x} be the unit vector in the x-direction and \hat{y} be the unit vector in the y-direction. Let $x(t)$ is the x-coordinate of the body at any instant of time and $y(t)$ the y-coordinate.

The net force acting on the body can be given as follows:

$$\vec{F} = \vec{F}_g + \vec{F}_d$$

$$\vec{F} = -mg\hat{y} - b|\vec{v}|\vec{v}$$

But, $\vec{v} = v_x\hat{x} + v_y\hat{y}$ and $|\vec{v}| = \sqrt{v_x^2 + v_y^2}$

Also, $v_x = \frac{dx}{dt} = x'$ and $v_y = \frac{dy}{dt} = y'$

$$\vec{F} = -b\sqrt{(x')^2 + (y')^2} \cdot x' \cdot \hat{x} + \left(-mg - b\sqrt{(x')^2 + (y')^2} \cdot y' \right) \cdot \hat{y}$$

The x-component of the force in the above equation can be equated to mx'' which tells us the force acting in the x-direction by Newton's second law and similarly, the y-component of the force in the above equation can be equated to my''

Once you equate these, you would get two second order differential equations that you must solve simultaneously to obtain the trajectory of the motion. The constant b for a spherical body can be given as follows:

$$b = \frac{1}{2}\rho\pi r^2 C_d$$

where ρ is the density of the fluid through which the body is moving, r is the radius of the body and C_d is the drag coefficient.

Now, let us solve a problem.

The stadium has gone wild as the game is down to the final ten minutes. It is the final of the 2014 FIFA World Cup and both the teams (Argentina and Germany) are yet to score. The mighty obstacle blocking the innumerable attacks by the Argentinian strikers is the 6ft 4inch tall German goalkeeper Manuel Neuer who is the best goalkeeper of the tournament so far. Neuer gets to take a goalkick and this goalkick may be crucial. Neuer with all his experience and superior techniques is able to launch the ball with an initial launch velocity of 30m/s. Say Neuer shoots the ball at an angle of 30° with respect to the ground. How far will the ball travel

before hitting the ground ? Players usually don't wait till the ball hits the ground as the opposition may get the control of the ball. Thus, players usually leap to get the possession of the ball with their heads or may receive it with their chests. Assuming that an average German footballer is 6ft tall, he can intercept the ball way before it hits the ground. Say he jumps and receives the ball at a height of 7ft from the ground, how far does the ball travel horizontally (along the x-axis) before being intercepted by a player ?

We know that in the absence of air friction, the optimal angle of launch (to get the maximum horizontal range) is 45° . Suppose Neuer hadn't taken the kick with a launch angle of 30° and you armed with these differential equations are given a chance to take the goalkick being in the shoes of Manuel Neuer. What is the optimal launch angle (in degrees) including air friction to shoot the ball farther away (maximum range) and increase the chances of nearing the opponent's goal (assuming the initial launch velocity is the same) [Optimal angle is usually between 30 to 45 degrees] ? Does the value of maximum range differ significantly when air friction is included as opposed to the ideal parabolic trajectory you learnt in college physics where air friction is neglected. If it does differ significantly, by how much ? Thus do you think inclusion of air friction in this case makes a difference in the analysis of the goalkick?

Say an amateur goalkeeper was to take the goalkick instead of Manuel Neuer and hence can produce an initial launch velocity of 25m/s. What will be the optimal launch angle and the maximum range for this goalkeeper?

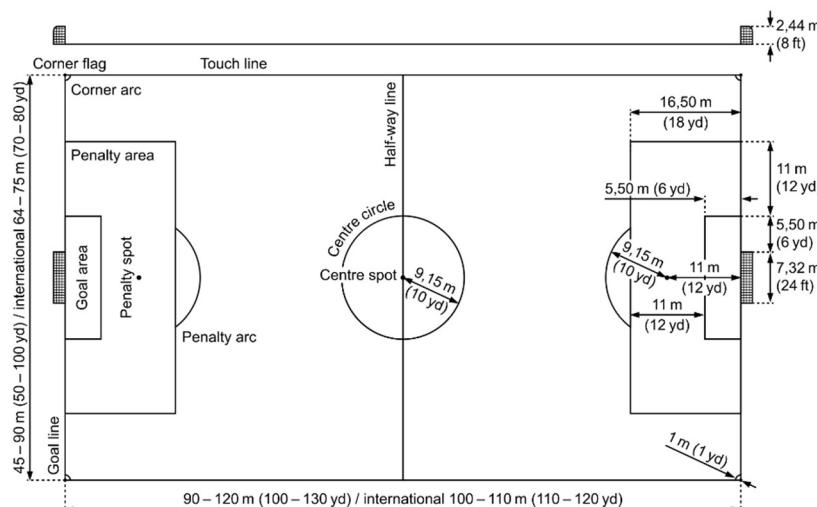
What do you conclude from the last question? How does the launch velocity affect the optimal angle of launch?

For the sake of this problem, you may assume that the ball doesn't curve and the trajectory can be treated as motion in 2-D (in reality, the ball may curve, wind speed and direction may play a role causing the motion to actually be in 3 dimensions). You may use the following data to solve the problem:

By FIFA standards, an official match ball weighs roughly 0.45kg and the radius of the ball can be taken as 0.11m. The drag coefficient can be roughly estimated to be 0.2

Density of air = 1.225 kg/m^3 , 1ft = 12 inches , 1ft = 0.3048m and $g = 9.8 \text{ m/s}^2$

Are the results of this exercise consistent with your observations of an actual goalkick? Given below is a schematic diagram of a football ground. Do you think the maximum range calculated by including air friction matches with your observation of roughly where a ball lands during goalkicks normally or is the ideal no friction case more relevant? (This question isn't graded, you may answer this to acknowledge how important the inclusion of air friction is in the calculations)



Though the width and length of the field varies from stadium to stadium as shown in the above diagram, Maracana Stadium (where the 2014 FIFA Final took place) has the most commonly used standard dimensions of $105\text{m} \times 68\text{m}$. You may use this data to answer the previous (ungraded) question.

[20 Marks]

- 3) You have intercepted a secret message encoded as a string of numbers. The message is **decoded** via the following mapping:

Where the numbers correspond to the English alphabet as follows:

"1" -> 'A'

"2" -> 'B'

...

"25" -> 'Y'

"26" -> 'Z'

However, while decoding the message, you realize that there are many different ways you can decode the message because some codes are contained in other codes ("2" and "5" vs "25").

For example, "11106" can be decoded into:

- "AAJF" with the grouping (1, 1, 10, 6)
- "KJF" with the grouping (11, 10, 6)
- The grouping (1, 11, 06) is invalid because **"06" is not a valid code** (only "6" is valid).

Note: there may be strings that are impossible to decode.

Given a string s containing only digits, return the **number of ways to decode** it along with the **possible hidden message**. If the entire string cannot be decoded in any valid way, return 0.

Sample→

Input: s = "226"

Output: 3

Explanation:

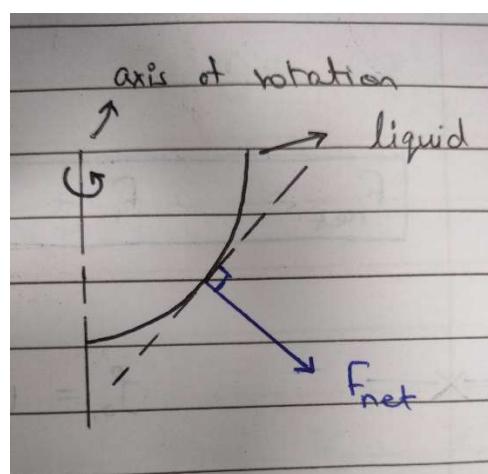
"226" could be decoded as "BZ" (2 26), "VF" (22 6), or "BBF" (2 2 6).

[8 marks]

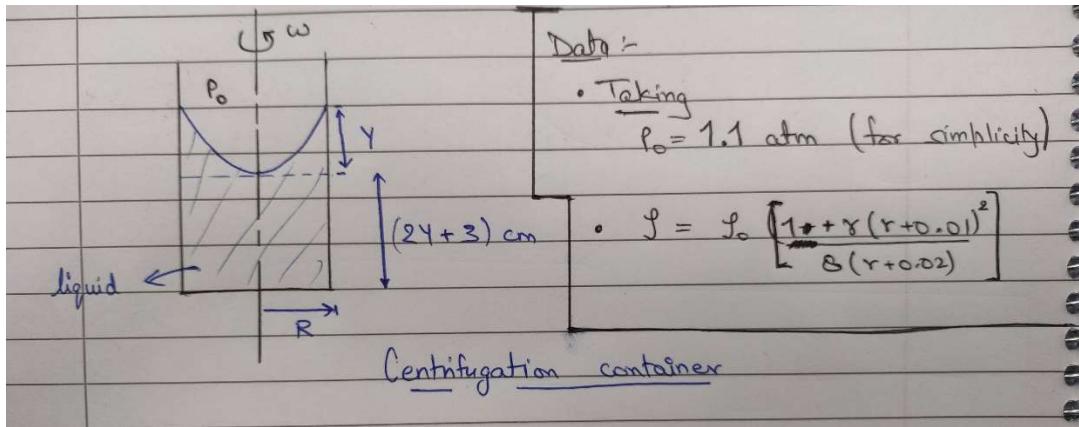
- 4) Centrifugation is a common industrial practice. Centrifugation uses centrifugal force to separate particles in suspension based on their size and density. There are different types of centrifuges, including low-speed, high-speed refrigerated, and ultracentrifuges. This technique is widely used in the pharmaceutical industry for various purposes like Drug purification, Vaccine production, Cell separation, etc... Due to the high speed of rotation of the container (containing liquid to be centrifuged), a density gradient is formed resulting out of variable mass distribution.

Due to the continuous rotation of the container at high velocity the top surface profile becomes **concave upwards**.

Concept: The net force acting on any part of the fluid is always perpendicular to the fluid's plane.



Schematic Diagram:



Data:-

Quantity	Values
rpm	3500
Diameter of container (cm)	3

Find the Net force at the bottom of the container?

[7 marks]

Use Computers but don't be a bot

Be Human, be creative