TECHNOLOGICAL UNIVERSITY DUBLIN
TALLAGHT CAMPUS

Bachelor of Science (Honours)

Pharmaceutical Science - Nanjing Joint Program

Full Time

Semester Seven : January 2023

Manufacturing Technology

Internal Examiners
Dr Adrienne Fleming
Dr Eugene Hickey

External Examiners
Dr Ken Kinsella

Day	**Wednesday**
Date	**4th January 2023**
Time	**09:30-11:45**

Instructions to Candidates

Section A: A Fleming: Answer any two out of the three questions.
Section B: E HIckey: Answer any two out of the three questions.

SECTION B: [Dr. Adrienne Fleming]

You are required to answer TWO complete questions

Question 1 – Answer all parts (100 marks)

a) What information does Reynolds number provide? What is the critical Reynolds number? (15 marks)

b) What problems can occur in chemical processing as a result of poor volume to surface areas. (15 marks)

c) An open straight blade turbine of 0.88m in diameter is used to stir reaction mixtures in a 20 m^3 batch reactor with baffles. The vessel diameter is 1.4m. The mixture is to be stirred at reflux. Addition of one of the reactants takes place into the agitator region. Given that the agitator speed has been fixed at 110rpm, determine the mixing time in seconds.
$Po=1.07$, $\mu = 0.012$ Ns m^{-2} ; $\rho=890$ kg m^{-3} (40 marks)

d) *"Batch processing rather than continuous processing is the traditional mode employed in the pharmaceutical manufacturing environment".* Discuss. (30 marks)

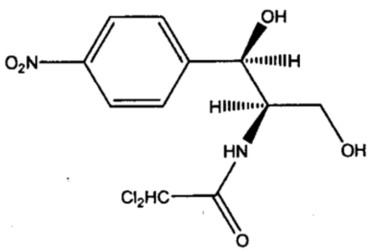
Question 2 – Answer all parts (100 marks)

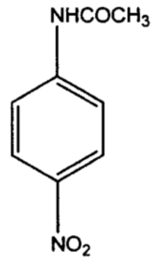
a) Using examples discuss 5 potential strategies utilized to make modifications to a chemical structure to alter its potency and activity. (25 marks)

b) Capital cost estimations can be classified into three broad categories'. Discuss each of these categories and their purpose. (20 marks)

c) A new plant is being designed for the production of an API. Given that the installation cost of a 10m3 reactor in year A has been calculated to be €125,000, predict the cost in year B, given the following CEI cost index data: CEI (A) = 420 and CEI (B) = 525 (30 marks)

d) Determine whether the following compounds have potential detonating properties based on their Oxygen Balance (25 marks)





Molecular Mass: 321.11 g/mole 180.16 g/mole
Chemical Formulas: $C_{11}H_{12}N_2Cl_2O_5$ $C_8H_8N_2O_3$

Question 3 – Answer all parts (100 marks)

a) Determine the rate of heat generation (in Watts, assuming Q calculated in J s^{-1}) from the reaction of 230 moles of reactant A with reactant B in water to be -25.4 kJ mol^{-1}. The activation energy was calculated as being 134 J mol^{-1} while the reaction rate constant was determined as being 3.2×10^{-4} s^{-1}

[R=8.314 J K^{-1} mol^{-1}] (30 marks)

b) A 20 m^3 batch reactor is fitted with a flat blade turbine agitator of diameter 1.4 m and is set to operate at 110 r/min. The reactor is to be used to react 7.5 moles of reactant A with reactant B at room temperature. The homogeneous reaction mixture has a density of 1856 kg m^{-3} and a viscosity of 1.4 Ns m^{-2} with a calculated rate constant of 3.02 s^{-1} . In this process reactant A is to be added in a controlled fashion down the walls of the vessel. Using time constant calculations determine whether product selectivity is determined by micromixing or reaction kinetics. [P0 = 0.98]. (40 marks)

c) Discuss the five root causes of waste in an API Plant. (10 marks)

d) Discuss the importance of the control of crystallisation the API to ensure the correct polymorphic form is produced. (20 marks)

SECTION B: [Dr. Eugene Hickey]

You are required to answer TWO complete questions

Question 4 **(100 marks)**

a) A feed stream goes into a distillation column with a feed flow of 118kg/hr and a composition of 25% octane, 45% heptane, 30% hexane. The distillate stream from the column carries 86% of the hexane fed and virtually no octane. The bottoms stream is 71% octane. Use this information to fill out the table below. (40 marks)

	Feed Stream	*Distillate Stream*	*Bottoms Stream*
Total Flow (*kg*/*hr*)			
Octane Flow (*kg*/*hr*)			
Heptane Flow (*kg*/*hr*)			
Hexane Flow (*kg*/*hr*)			
Octane Percent (%)	%	%	%
Heptane Percent (%)	%	%	%
Hexane Percent (%)	%	%	%

b) 10% excess air is supplied to a furnace burning 100m^3/hr of natural gas (95% methane, 5% ethane by volume). Calculate the air flow of air (21% O_2) required. The reactions are:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$C_2H_6 + 7/2\ O_2 \rightarrow 2CO_2 + 3H_2O$$

(20 marks)

c) A compound crystallises in BCC. The molecular weight is 145.8g/mol. If the density is 1.829g/cm^3, calculate the lattice parameter in nm. Avogadro's number is 6.022×10^{23}. (15 marks)

d) An FCC crystal is made from ions of radius 0.26nm. Calculate the lattice parameter in nm. (15 marks)

e) A unit cell has parameters a=1.54nm, b=4.18nm, and c=2.25nm. It has angles $\alpha = 90^0$, $\beta = 94.3^0$, and $\gamma = 90^0$. What is the shape of the unit cell? (10 marks)

Question 5 **(100 marks)**

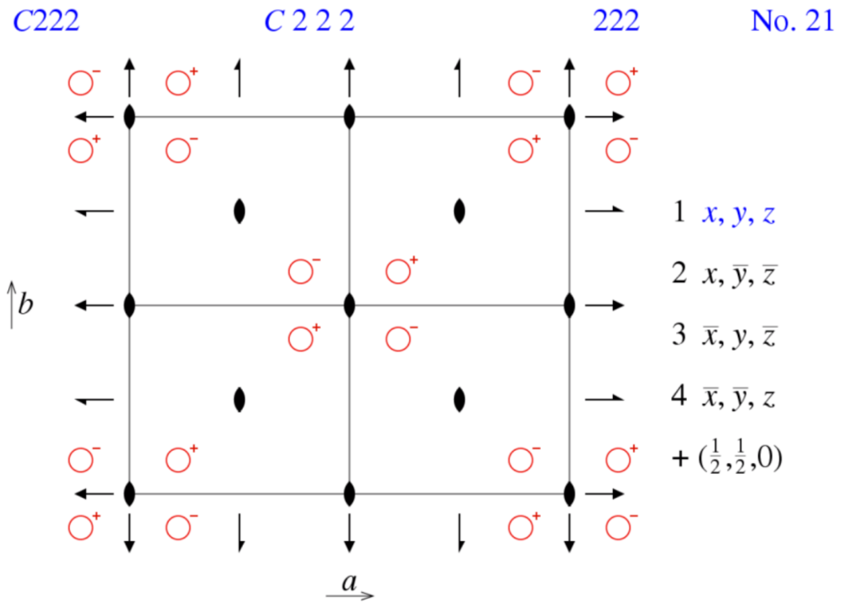
e) An oil stream enters a counter flow heat exchanger at a temperature of $95°\mathrm{C}$ and leaves at $56°\mathrm{C}$. The cold stream has an input temperature of $11°\mathrm{C}$ and an output temperature of $46°\mathrm{C}$. The flow of the hot stream is $3.1\mathrm{kg/s}$. The heat capacity of the hot stream is = $1160\mathrm{J/kg/°C}$

(i) Show that the flow of heat across the heat exchanger is 140.2kJ/s (15 marks)

(ii) Show that the LMTD for this process is 47°C. (10 marks)

(iii) Calculate the UA value of the heat exchanger. (15 marks)

f) The diagram below shows the orthorhombic space group, C222



(i) What does orthorhombic mean in terms of the length of the three sides, a, b, c, and the angles between them, α, ß, and γ? (10 marks)

(ii) Is this space group Primitive, Face Centred, Body Centred, or Base Centred? (5 marks)

(iii) What does **222** mean in the space group title? (10 marks)

(iv) Is there a centre of symmetry in the cell? Justify your answer. (10 marks)

(v) What is the multiplicity of the general position, (x, y, z), for the space group? (10 marks)

(vi) What kind of symmetry is denoted by the  symbol in the diagram above? (10 marks)

(vii) What kind of symmetry is denoted by the  symbol in the diagram above? (5 marks)

Question 6 (100 marks)

a) The diagram below shows a vapour liquid equilibrium (vle) diagram for a mixture of acetone and benzene at 101.3kPa. Explain what is plotted on the x and y axes of a vle diagram? (5 marks)

b) Explain how a vle diagram can be constructed from a binary phase diagram (10 marks)

c) Use the diagram to answer the following questions:

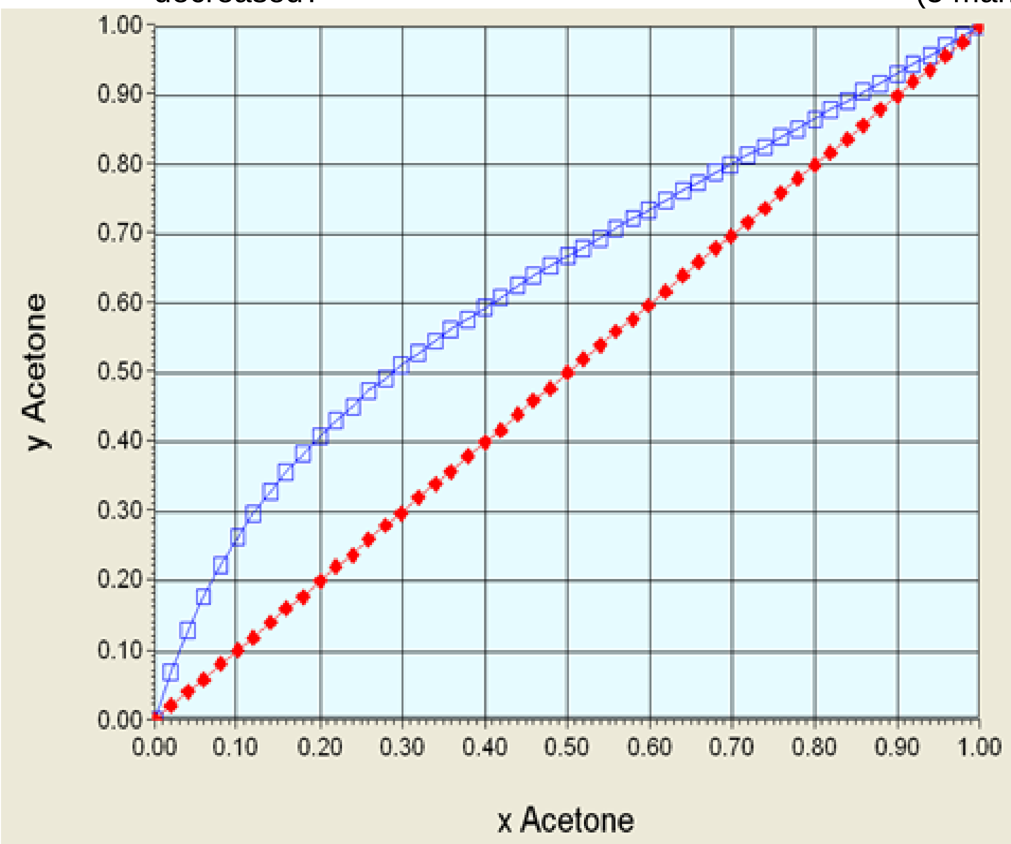
(i) What is the mole fraction in acetone of the vapour phase when the mole fraction in acetone of the liquid phase is 0.6? (5 marks)

(ii) What is the mole fraction in acetone of the liquid phase when the mole fraction in benzene of the vapour phase is 0.2? (5 marks)

(iii) What is the mole fraction in benzene of the liquid phase when the mole fraction in benzene of the vapour phase is 0.7? (5 marks)

(iv) Calculate the relative volatility of acetone in benzene when the liquid mole fraction of acetone is 0.5 (15 marks)

(v) What would happen to this vle curve if the pressure was decreased? (5 marks)



[QUESTION 6 CONTINUED OVERLEAF]

d) The Bragg Equation gives the conditions for coherent scattering of x-rays from a crystal lattice, It is written as: $n\lambda = 2d \sin \theta$. Explain the different terms in this equation. (5 marks)

e) CuKα radiation ($\lambda = 0.154051$nm) is incident on a powder crystal sample. It produces a first order diffraction peak at $2\Theta = 40.7°$. What is the corresponding interplanar spacing, d? Please give your answer in nm to three significant figures. (15 marks)

f) A tetragonal lattice has lattice parameters of a = b = 3.867nm and c = 1.975nm. What is the interplanar spacing in nm of the (hkl) = (4 1 3) planes? (15 marks)

g) X-ray diffraction on a cubic crystal reveals peaks at (6 2 6), (0 0 6), (7 7 1), and (7 1 1). There are no peaks observed at (6 1 0) or (7 6 1). What type of Bravais lattice is this? (15 marks)

LIST OF FORMULAE

$$t = \frac{-1}{k \ln(1 - x_A)}$$

$\tau_R = 1/kC_{A0}$

$\tau_R = 1 + a/kC_{A0}$ where $a = V_A / V_B$

$$Re = \frac{\rho v D}{\mu}$$

$$Re = \frac{\rho N D^2}{\mu}$$

$P = P_0 N^3 D_A^5 \rho$

$\varepsilon_{mean} = P / V\rho$

$Re_c = 6370 / P_0^{1/3}$

$P_0^{1/3}\ Re\ Fo = 5.2$

$$Fo = \frac{\mu t_{95}}{\rho T^2}$$

The lifetime of an Eddy is τ_K:

$$\tau_K = 12[\upsilon / \varepsilon]^{1/2}$$

where $\upsilon = \mu / \rho$ (kinematic viscosity)

Engulfment Rate E = $\ln 2 / \tau_K$

$\tau_E = 1/E$

$$C_2 = C_2 \left(\frac{S_2}{S_1}\right)^n$$

C_2 = capital cost of project with capacity S_2
C_1 = capital cost of project with capacity S_1

$$D = \frac{C}{10\ x\ V}$$

D = depreciation in €/kg
C = capital cost in €
V = production volume in kg/year
10 is the plant life

$Q_r = V(-\Delta H_r)k_0 C_A \exp(-E_A/RT)$

$Q_c = UA(T-T_a)$

$MTSR = T_p + \Delta T_{ad}$

$\Delta T_{ad} = \Delta H.n / m.C_p$

$TMR_{ad} = C_p RT^2 / q_0 E_A$

$$\text{Oxygen balance} = \frac{-[1600(2a + b/2 - c)]}{\text{Mol. Wgt.}}$$

$q = mc\Delta T$

$q = UA\ LMTD$

$$LMTD = \frac{\Delta T_L - \Delta T_R}{\log_e(\Delta T_L / \Delta T_R)}$$

Molar mass CO_2 = 44g/mol

Molar Mass Air = 29g/mol

$n\lambda = 2d \sin\theta$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

$\lambda_{Cu\,K_\alpha}$ = 0.154051nm

$$\alpha_{AB} = \frac{y_A / x_A}{y_B / x_B}$$

q = liquid fraction

$$slope = \frac{-q}{1-q}$$

q-line goes between (x_F, y_F) and (0,x_F/(1-q))

rectifying line between (x_D, y_D) and (0,x_D/(R+1))

F = D + B

F x_F = Dx_D + B