National Exams May 2019

16-Chem-B10, Life Cycle Assessment (LCA)

3 hours duration

NOTES:

1. If doubt exists as to the interpretation of any question, the candidate is urged to submit with the answer paper a clear statement of any assumptions made.

2. This is a CLOSED BOOK EXAM.
   One of two calculators is permitted – any Casio or Sharp approved model. One double-sided aid sheet is permitted.

3. Question 1 MUST be completed. Any THREE (3) of the remaining four questions (i.e. Questions 2 to 5) constitute a complete exam paper. Only the first four questions as they appear in the answer book will be marked.

4. 28 marks are for Question 1, and 24 marks for each of Questions 2 to 5. Marks for question parts are indicated beside each question (i.e. [10], [5], etc.)

5. Most questions require an answer in essay format. Clarity and organization of the answer are important.

MANDATORY: Question 1 MUST be completed

Question 1 (28 Marks) Life Cycle Analysis

[10] (a) Life cycle analysis (LCA) of a process or a product requires the input from many people with different educational backgrounds and experiences. List and describe the different perspectives required to create an effective LCA for a product or a process.

[6] (b) Describe the possible effects of a) unclear system boundaries and b) functional units on life cycle analysis (LCA) comparison studies. Provide a theoretical examples for the effects of a) unclear system boundaries and b) unclear functional units.

[6] (c) Risks are associated with all processes and all waste effluents. Describe the generalized components used to estimate the risk for

i) an operating chemical process, and

ii) producing an aqueous waste effluent.

Provide theoretical examples of risk evaluations for a unit operation, and an aqueous or gaseous effluent stream of your choice. List any assumptions you make regarding the nature and severity of the example risks for cases i) and ii).

[6] (d) Ammonia, CFC's, and HFC's are three families of refrigerants with different ozone depletion potentials. Briefly describe, compare, and contrast more than one environmental and safety concerns associated with each of these families of compounds.

REMAINDER: Answer THREE (3) of the next four (4) questions. Be sure to indicate the question number in your Answer Paper.

Question 2 (24 Marks) Tier 1 Economic and Performance Evaluation

There are two chemical processing routes for the production of toluene diisocyanate (TDI, MW 174.2 g/mol, ρ=1.214 g/cm^3). TDI is used in the production of polyurethane. The two processing routes are:

1) reaction of toluenediamine ($C_6H_3(CH_3)(NH_2)_2$) with phosgene ($COCl_2$) in a chlorobenzene solvent, and
2) carbonylation of dinitrotoluene ($C_6H_3(CH_3)(NO_2)_2$) with carbon monoxide (CO) over a mixed oxide catalyst in a chlorobenzene and pyridine solvent.

The chemical reactions for each processing rout are:

Process 1) $C_6H_3(CH_3)(NH_2)_2 + 2\ COCl_2 \rightarrow C_6H_3(CH_3)(-N=C=O)_2 + 4\ HCl$

Process 2) $C_6H_3(CH_3)(NO_2)_2 + 6\ CO \rightarrow C_6H_3(CH_3)(-N=C=O)_2 + 4\ CO_2$

The first process (carbonylation of dinitrotoluene) has been proven in the laboratory, but has not been scaled up to pilot production scale. Initial data suggest 100 % conversion of dinitrotoluene, with TDI selectivity of 70-95 %. Approximate stoichiometric data, and 1996 chemical costs, are in Table 1.

Table 1: Stoichiometric data for two TDI production processes.

Compound	Lbs produced / lbs raw material required per lb TDI*	Cost ($/lb)**	PEL (mg/m^3)	Overall inhalation toxicity factor	Overall oral toxicity factor
Amine-phosgene route (Process 1)					
phosgene	-1.26	0.610	0.4	NA	NA
toluenediamine	-0.76	0.576	0.1 (estimated)	NA	NA
chlorobenzene	-0.01	0.550	350	100	100
hydrochloric acid	0.4 (estimated)	0.027	7	100	100
TDI	1.00	1.34	0.14	100,000	100
Carbonylation route (Process 2)					
dinitrotoluene	-1.04 (estimated)	0.365	1.5	1,000	1,000
carbon monoxide	-1.0 (estimated)	0.040	55	NA	NA
solvent	-0.01	0.550	350	100	100
TDI	1.00	1.340	0.14	100,000	100
carbon dioxide	1.0 (estimated)	-	9000	NA	NA

* a negative value indicates a reagent; positive indicates a product.

** Chang, D., M.S. Thesis, UCLA, 1996

(continued on the next page)

Tier 1 economic analyses are estimated with Equation 2-1, and environmental index estimates are made with Equations 2-1 and 2-2

$$Economic\ Index = \sum[(|\nu_i| \times raw\ materials\ cost) - (|\nu_i| \times salable\ byproducts\ cost)] \quad \text{Eq. 2-1}$$

$$TLC\ Environmental\ Index = \sum |\nu_i| \times \frac{1}{TLV_i} \quad \text{Eq. 2-2}$$

$$EPA\ Environmental\ Index = \sum |\nu_i| \times maximum\ of\ oral\ and\ inhalation\ toxicity\ factor \quad \text{Eq. 2-3}$$

Where:

- TLV is the threshold limit value set by the American Conference of Governmental Industrial Hygienists (ACGIH).
- A similar concept to the TLV is referred to as the "permissible exposure limit (PEL) by another governmental agency, the United States Occupational Safety and Health Administration (OSHA).
- $|\nu_i|$ is the absolute value of the stoichiometric (by mass) coefficient of reactant or product i
- TLV_i is the threshold limit value (ppm) of reactant or product i,
- the sum is over all of the reactants and products of interest.

[12] Compare these two TDI production processes using Tier 1 economic and environmental performance evaluations.

[6] Provide and justify your recommendation of which process you would recommend for TDI production with your Tier 1 economic and environmental performance evaluations.

[4] List the limitations and assumptions used to support your recommendations.

[2] Explain why the TLV or PEL is an oversimplification of overall human health effects of chemical "exposure".

Question 3 (24 Marks) Estimation of Contaminant Effects

A golf course uses a pond on its grounds to raise trout for the golf club restaurant. The golf course uses 2,4 dichlorophenoxyacetic acid (2,4-D) as a herbicide to reduce weed growth.
During a recent herbicide application on the golf course, 100 g of 2,4-D was accidentally sprayed in the pond. The estimated volume of the pond is 1.5 million litres. It is assumed that there is significant sediment on the bottom surface of the pond.

The following properties for 2,4-D n-butyl ester were obtained from the US EPA property estimation program, EPIWIN:
Molecular weight: 221.04 g/mol
Log Kow: 2.41
Maximum water solubility: 336.2 mg/L (25 °C)
Lethal dose that kills 50 % of a life form in a given time (LD_{50}): 590 µmol/L

The following are estimates of properties of the pond:
Organic solids concentration in suspended sediment: 50 mg / kg water
Biota concentration: 75 g per 100 m^3 water
Soil sorption coefficient: 150 kg in soil / kg in water

Equations 3-1 and 3-2 are proposed estimation relationships:

$$LC_{50}\ for\ guppies: \log\left(\frac{1}{LC_{50}}\right) = 0.871 \log K_{ow} - 4.87 \qquad \text{Eq. 3-1}$$

$$\log BCF = 0.79\ (\log K_{ow}) - 0.40 \qquad \text{Eq. 3-2}$$

[3] (a) Explain in your own words the meaning of bioaccumulation potential, also known as bioconcentration factor (BCF).

[2] (b) What data from the EPIWIN estimated data set can you use estimate the bioaccumulation potential for 2,4-D and why?

[3] (c) What is your estimation of the bioaccumulation potential for 2,4-D?

[2] (d) Determine the LD_{50} for trout in this pond, using guppies as a surrogate fish for the trout.

[2] (e) Was the LC_{50} exceeded after the recent herbicide contamination in the pond?

[12] (f) Estimate the amount of 2,4D that would be ingested if a golfer were to consume 0.25 kg of trout fish tacos made at the golf club with fist from this pond, after the herbicide application. State your assumptions that apply to your calculations.

Question 4 (24 Marks) Life Cycle Analysis

Perform a streamlined LCA *comparison* on one of the following topics:

i) plastic water bottle for personal use versus a portable metal water bottle for personal use, both with plastic caps,
ii) any two of: paper grocery-carrying bag versus, single use plastic carrying bag, or a reinforced, multiple-use plastic carrying bag,
iii) hydroelectric power plant versus natural gas-fired power plants,
iv) personal use automobile with an electric motor versus personal use automobile with a gasoline engine, considering the fuel that electrifies the power grid.

This is a broad-based essay-style question, with a length reflective of the relative marks assigned (expect to spend ~ ¼ of the exam length on this question).

Your response will be evaluated based on the following components of your answer:

[5] Topic description, identification of suitable system boundaries, and appropriate selection of functional units and targeted outcome of your comparison.

[15] Application of engineering judgment in the scope of the system inventory and assignment and evaluation of impact factors. Breadth of discussion and depth of understanding of the selected topic. While numerical values of variables relevant to the comparison are not expected, relative assessments and identification of affected systems are required.

[4] Organization, legibility, cohesiveness of response.

Your response will be assessed on the quality of your analysis process and your ability to provide an impartial assessment, not based on your final comparative conclusions.

Question 5 (24 Marks) Sustainable Engineering Practice

Answer THREE (3) of the following five questions. Only the first three answered questions will be marked:

[8] (a) Discuss the principles, risks, and advantages of a network of companies connected through an Industrial Ecology model.

[8] (b) Briefly describe the purposes and results for a Tier 1, Tier 2 and Tier 3 environmental assessment of an industrial process. In what development stage is each Tier assessment undertaken, and why?

[8] (c) In the context of workplace health and safety, list the routes of chemical exposure for workers. Explain if and how it is possible for one toxic compound to have a lower toxicity dose that affects 10% of a species (TD_{10}) and a toxicity dose that affects 50% of a species (TD_{50}) than a second compound.

[8] (d) What is an "Environmental Release Assessment" for an industrial process? List the environmental components that can be affected by an industrial, environmental release. List and explain the chemical and physical properties of a contaminant that will affect its transport into the environmental components.

[8] (e) Discuss the roles of engineers, companies, regulators, and other related governmental agencies on the actions required to increase the sustainability of an industry of your choice.