2105623 Optimization of Chemical Processes

Department of Chemical Engineering, Chulalongkorn University

Homework 1: Linear and Network Model Construction

Semester 1/2026 | Covers Weeks 1–3 | Released Week 2, due Week 4 class

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Instructions. Work individually. This set is deliberately formulation-heavy: most of the credit is for a correct, complete and clearly defined model, not for arithmetic. For every problem, state the index sets, the decision variables *with units*, the objective function and all constraints in explicit algebraic form. Where a problem asks for a classification, name the model class (LP, IP, MILP, NLP, MINLP), state whether it is continuous or mixed-integer, and state whether it is deterministic or stochastic. Numerical answers must be accompanied by the reasoning that produced them. Submit one PDF plus, for Problem 5, one runnable `.py` file. Total: 100 points.

Problem 1. Multiperiod production planning with inventory (24 points)

A plant produces gas-diffusion electrodes for zinc-air batteries. Planning is done over the four months $t = 1, \ldots, 4$ of a delivery contract. The contracted demand, which must be met in full in the month in which it falls due, is

Month t	1	2	3	4
Demand d_t (tonne)	200	260	310	230

Each month the plant can produce up to 240 tonne on regular time at a cost of 30 thousand baht per tonne, and up to a further 60 tonne on overtime at a cost of 48 thousand baht per tonne. Electrode material held at the end of a month incurs a controlled-atmosphere storage charge of 4 thousand baht per tonne per month. The opening inventory is 30 tonne and the contract requires a closing inventory of at least 20 tonne at the end of month 4. Backorders are not permitted.

(a) Define the index set, the parameters and the decision variables, with units.

(b) Write the inventory balance constraint for a general period t, taking care of the first period. State explicitly which quantity in that constraint is a datum and which is a variable.

(c) Write the capacity constraints, the closing inventory requirement and the sign restrictions. Identify the single restriction that forbids backorders.

(d) Write the total cost objective function.

(e) Sum the four balance equations. Show that the total quantity produced over the horizon is fixed by the data, compute that quantity, compare it with the total available capacity, and state whether the model is feasible.

(f) Classify the model. Then explain, using the cost data, why it can be optimal to hold inventory even though storage is not free. Support the explanation with an explicit cost comparison.

Problem 2. Transshipment in a lithium hydroxide supply chain (22 points)

Battery-grade lithium hydroxide is produced at two refineries, R_1 and R_2, with monthly capacities of 90 and 110 tonne. All output is first railed to one of two coastal ports, P_1 and P_2, and is then shipped from the ports to three cell plants, G_1, G_2 and G_3, whose monthly requirements are 60, 80 and 50 tonne. Nothing is held at a port from one month to the next. Transport costs in thousand baht per tonne are

Refinery to port	P_1	P_2	Port to plant	G_1	G_2	G_3
R_1	3	7	P_1	4	6	9
R_2	6	4	P_2	8	5	6

(a) Define the two families of decision variables and write the complete algebraic model: capacity constraints at the refineries, flow conservation at the ports, requirement constraints at the cell plants, and the total transport cost objective. State why the port constraint is an equality.

(b) State whether total supply equals total demand. If it does not, explain how this model absorbs the imbalance without introducing a dummy node, and state the one modelling choice that makes that possible.

(c) A logistics planner proposes the following schedule: $R_1 \to P_1 = 90$, $R_2 \to P_1 = 10$, $R_2 \to P_2 = 90$, $P_1 \to G_1 = 60$, $P_1 \to G_2 = 40$, $P_2 \to G_2 = 40$, $P_2 \to G_3 = 50$, all other flows zero. Verify every constraint and compute the total monthly cost of this schedule.

(d) Classify the model. All capacity, requirement and cost data are integers. State what can therefore be said about the optimal values of the flow variables, and name the structural property of the constraint matrix that guarantees it.

Problem 3. Process superstructure with continuous route splits (22 points)

A recycling plant receives $F = 120$ tonne per day of black mass recovered from spent lithium-ion cells. The whole stream must be processed on the day it arrives; it cannot be stored or discarded. Two alternative recovery routes are available and the feed may be split between them in any continuous proportion.

Route	A (pyro-hydrometallurgical)	B (direct hydrometallur
Product yield η_k (t product per t feed)	0.80	0.90
Operating cost w_k (thousand baht per t feed)	12	18
Throughput limit U_k (t feed per day)	80	70
Product purity π_k (mass fraction)	0.960	0.995

The two product streams are combined into a single mixed-sulfate product that is sold at 30 thousand baht per tonne. The purity of the combined product blends linearly on a mass basis and must be at least 0.975.

(a) Let x_A and x_B be the feed rates sent to the two routes, in tonne per day. Write the feed balance, the throughput limits, the product balance and the daily profit objective.

(b) The purity requirement is naturally written as the ratio

$$\frac{\sum_k \pi_k \eta_k x_k}{\sum_k \eta_k x_k} \;\geq\; 0.975.$$

Show how to convert it into a linear constraint, state the condition under which the conversion is valid, and simplify the result to a single inequality in x_A and x_B.

(c) Define the split fraction $\theta = x_A/F$ and rewrite the model in terms of θ. Then suppose the daily feed F becomes a decision variable rather than a datum. Show which terms of the θ-model become products of two variables, name the resulting model class, and state which of the two equivalent formulations, the flow form or the split-fraction form, should be given to a solver.

(d) Solve the base instance ($F = 120$) by hand. Report the optimal split, the daily product rate, the delivered purity, the daily profit, and which constraints are active.

Problem 4. Classification of problem types (12 points)

Classify each of the following models using exactly one label from {LP, IP, MILP, NLP, MINLP}. For each one, give a single sentence that names the feature responsible for the classification, and state whether the feasible region is convex.

(i) Minimizing the total operating cost of a multiperiod production plan in which all costs are linear and production, inventory and shipment quantities are continuous.

(ii) Choosing which of five candidate electrolyzer sites to construct and, simultaneously, the continuous tonnages shipped on every route, with linear construction and transport costs.

(iii) Estimating the two continuous parameters of a Langmuir adsorption isotherm by minimizing the sum of squared residuals against 30 laboratory measurements.

(iv) Deciding how many identical vanadium redox flow battery stacks, an integer count, to install at each of four substations, subject to a linear capital budget and linear energy requirements.

(v) Selecting the reactor temperature and the catalyst loading, both continuous, together with the number of reactors in series, an integer, so as to minimize a nonlinear annualized cost.

(vi) Blending three feed streams that first pass through a common surge drum, so that every product drawn from the drum has the same unknown composition, with continuous flows and linear costs.

Problem 5. Pyomo implementation of the transshipment network (20 points)

Implement the transshipment model of Problem 2 in Pyomo as a `ConcreteModel`.

(a) Build the model over an *arc set*: declare a `Set` of nodes, a `Set` of directed arcs initialized from a list of tuples, and a `Param` indexed by that arc set holding the unit costs. Declare one `Var` indexed by the arc set. Write the supply, conservation and requirement constraints as rules over the node sets. No datum may be hard-coded inside a constraint rule.

(b) Solve with any available linear solver (`appsi_highs`, `glpk` or `cbc`) and include an explicit assertion on the termination condition.

(c) Report the optimal cost and a table of every arc carrying positive flow. Confirm that the optimal flows are integers and connect this to your answer to Problem 2(d).

(d) Scenario 1. Port P_1 is placed under a throughput limit of 60 tonne per month. Add the single constraint that expresses this, re-solve, and report the new optimal cost and routing. State the cost of the restriction in thousand baht per month.

(e) Scenario 2. Starting again from the base data, a new direct rail link $R_2 \to G_3$ becomes available at 9 thousand baht per tonne, bypassing the ports. Add the arc to the data only, with no change to any constraint rule, re-solve, and report the new optimal cost and routing.

Submit the script and its printed output. The script must run top to bottom without manual input.

Grading Rubric (Total: 100 points)

1. Multiperiod production planning (24 pts)

- Sets, parameters, variables with units (4)
- Inventory balance, first period handled correctly (5)
- Capacity, closing inventory, sign restrictions, backorder statement (4)
- Cost objective (3)
- Aggregate balance, required production, feasibility check (5)
- Classification and cost-based justification of holding stock (3)

2. Transshipment network (22 pts)

- Variables and complete algebraic model, port equality justified (8)
- Supply and demand imbalance discussion (3)
- Feasibility check and cost of the proposed schedule (6)
- Classification and total unimodularity argument (5)

3. Process superstructure (22 pts)

- Balances, throughput limits and profit objective (6)
- Linearization of the purity ratio with validity condition (5)
- Split-fraction form, bilinearity when F is a variable, formulation choice (5)
- Correct optimal split, product rate, purity, profit, active constraints (6)

4. Classification of problem types (12 pts)

- Six items, 2 points each: 1 for the label, 1 for the reason and the convexity verdict (12)

5. **Pyomo implementation (20 pts)**
   - Arc-set model structure with named components and `Param` data (7)
   - Solve, termination assertion and correct base cost (5)
   - Flow table and integrality comment (3)
   - Scenario 1 correctly reported and costed (3)
   - Scenario 2 correctly reported (2)

Reference. Rao, *Engineering Optimization: Theory and Practice*, 4th ed., Ch. 1; Williams, *Model Building in Mathematical Programming*, Ch. 3 and Ch. 5.