2105623 Optimization of Chemical Processes

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Homework 2: Blending, Pooling, Logical and Discrete Modeling

Semester 1/2026 | Covers Weeks 4–6 | Released Week 4, due Week 6 class

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Instructions. Work individually. State every decision variable with its units before using it. Wherever a big-M coefficient appears you must give the *smallest* value of M that is valid and justify it from the bounds on the variables involved; a formulation with an unjustified M receives at most half credit. Problem 6 is a model audit and must be answered from the printed listing: you may run the code to confirm your findings, but the reasoning, not the output, is what is graded. Total: 100 points.

Problem 1. Blending with quality specifications (20 points)

Part A (general formulation). A plant blends a set I of solvent streams into a set K of finished battery electrolytes. Stream i is available at up to a_i L/h, costs c_i baht per litre, has conductivity index κ_i and water content w_i ppm. Electrolyte k must be produced at exactly Q_k L/h, must have a conductivity index of at least $\underline{\kappa}_k$ and a water content of at most $\bar{w}_k$ ppm. Both properties blend linearly on a volume basis.

(a) Define the decision variables x_{ik} and write the production, availability and quality constraints together with the cost objective. State the model class.

Part B (numerical instance). A single electrolyte grade is produced at exactly 400 L/h from three streams:

Stream	Cost (baht/L)	Conductivity κ_i	Water w_i (ppm)	Available a_i (L/h)
EC-rich carbonate (E)	40	12	15	300
DMC-rich carbonate (D)	25	8	30	240
Additive concentrate (A)	90	24	5	120

The grade must have a conductivity index of at least 12 and a water content of at most 17 ppm.

(b) Write the three-variable linear program explicitly, with the quality constraints already in unnormalized (multiplied-through) form.

(c) Eliminate one variable using the volume balance, reduce the problem to two variables, and solve it. Report the optimal blend, the hourly cost, the delivered conductivity index and the delivered water content.

(d) State which constraints are active at the optimum and which are slack, and say what the slack ones imply about their shadow prices.

Problem 2. Ratio-constraint linearization (10 points)

(a) A requirement has the form $(\alpha^\top x)/(\beta^\top x) \le \gamma$. State the linear constraint that is equivalent to it and the condition on the denominator under which the equivalence holds.

(b) Using the instance of Problem 1 Part B, write "stream D must make up at least 20 percent of the blend by volume" as a linear constraint.

(c) Write "the volume of E must be at least three times the volume of D" as a linear constraint.

(d) State two distinct situations in which multiplying through by the denominator is *not* valid, and say what the linear form becomes in each case (an equivalent, a relaxation, or a restriction).

(e) Add the constraint of part (b) to the instance of Problem 1 Part B and re-solve. Report the new blend, the new hourly cost, and the cost of the restriction.

Problem 3. A pooling problem and why it is nonconvex (18 points)

Two recovered solvent streams are collected in a common surge drum before use. Stream 1 contains 300 ppm water and costs 20 baht/L; stream 2 contains 100 ppm water and costs 34 baht/L. Let $F_1, F_2 \ge 0$ be the flows into the drum in L/h. The drum is perfectly mixed, so everything drawn from it has the same unknown water content p ppm, with $100 \le p \le 300$. The drum feeds two products:

Product	Water specification	Price (baht/L)	Maximum sales (L/h)
X (industrial grade)	at most 250 ppm	40	100
Y (battery grade)	at most 150 ppm	50	60

Let $P_X, P_Y \geq 0$ be the flows drawn from the drum to products X and Y, in L/h. Nothing accumulates in the drum.

(a) Write the complete model: the drum mass balance, the drum water balance, the two product specifications, the sales limits and the profit objective. List every term that is a product of two decision variables.

(b) The water specification for product X can be written as the ratio $(pP_X)/P_X \leq 250$. Explain why multiplying through by the denominator, which removed the nonlinearity in Problem 2, does *not* remove it here. Identify precisely which balance the troublesome denominator belongs to.

(c) Verify that the two points

$$\text{(i)} \quad p = 150,\ F_1 = 40,\ F_2 = 120,\ P_X = 100,\ P_Y = 60,$$

$$\text{(ii)} \quad p = 250,\ F_1 = 75,\ F_2 = 25,\ P_X = 100,\ P_Y = 0$$

are both feasible. Then form their midpoint and show that it is infeasible, giving two separate reasons. State what this proves about the feasible set and why it matters for the solver you would choose.

(d) Fixing p at a number turns the model into a linear program. Solve that linear program by hand for $p = 150$ and for $p = 250$, and report the profit in each case. Explain what a local gradient-based solver started near $p = 300$ would report, and what it would fail to report.

Problem 4. Big-M selection with the tightest valid constant (16 points)

A hydrogen distribution company must supply $D = 520$ tonne per month from up to four candidate production sites $j = 1, \ldots, 4$:

Site j	1	2	3	4
Fixed cost F_j (thousand baht/month)	2400	1800	3000	2100
Variable cost c_j (thousand baht/tonne)	34	40	28	36
Capacity U_j (tonne/month)	180	150	260	200

Let $x_j \geq 0$ be the monthly output of site j and $y_j \in \{0, 1\}$ equal 1 if site j is built.

(a) Write the fixed-charge linking constraint. Derive the smallest valid M_j for each site from the two bounds that apply to x_j, and give the four numbers.

(b) A built site must operate at no less than 60 tonne per month, and a site that is not built produces nothing. Write this, and state whether a big-M constant is needed.

(c) Write each of the following as a linear constraint in the y_j: (i) site 3 may be built only if site 1 is built; (ii) at most three sites may be built; (iii) sites 2 and 4 may not both be built.

(d) Either site 1 produces at least 120 tonne per month or site 4 produces at least 120 tonne per month, or both. Introduce the necessary binary variable, write the pair of constraints, and give the tightest valid value of each big-M with its justification.

(e) Consider only the fixed-charge constraints of part (a), the capacity bounds $x_j \leq U_j$, the demand constraint $\sum_j x_j \geq D$ and the objective $\min \sum_j (F_j y_j + c_j x_j)$. Solve the mixed-integer program, then solve its linear programming relaxation twice: once with the tight M_j of part (a) and once with $M_j = 100\,000$ for every j. Report the three objective values and the two relaxation gaps as a percentage of the integer optimum, and state in one sentence what this demonstrates about the choice of M.

Problem 5. Convex hull versus big-M: comparing relaxation bounds (16 points)

A pilot unit is fed with two raw materials at rates x_1 and x_2 tonne per hour, and the contribution margin is $2x_1 + 3x_2$ thousand baht per hour, to be maximized. Global equipment limits give $0 \leq x_1 \leq 6$ and $0 \leq x_2 \leq 6$. Exactly one of two operating technologies must be selected, and the choice imposes a different pair of process limits:

$$\text{Technology } A: \quad x_1 + x_2 \leq 6, \quad x_1 \leq 4 \quad \text{or} \quad \text{Technology } B: \quad x_1 + 3x_2 \leq 9, \quad x_2 \leq 2.$$

(a) Write the big-M formulation using a single binary y, with $y = 1$ selecting technology A. Derive the tightest valid M for each of the four process constraints from the global bounds, and give the four numbers.

(b) Write the convex hull (disaggregated) formulation: split x into $x^A + x^B$, introduce $y_A + y_B = 1$, and write every constraint of each disjunct scaled by its own binary, including the scaled global bounds.

(c) Solve the problem exactly by optimizing over each technology separately, and report the mixed-integer optimum with the selected technology.

(d) Consider the point $x_1 = 4$, $x_2 = 4$ with $y = 1/2$. Show that it satisfies every constraint of the big-M relaxation and compute its objective value. Then prove that it cannot lie in the convex hull of the two disjuncts by exhibiting a single inequality that is valid for technology A, valid for technology B, and violated by this point. State which relaxation is tighter and why that matters for branch and bound.

Problem 6. Model audit (20 points)

An engineer asked a language model to write a Pyomo model for the specification below and received the listing on the next page. It is syntactically correct, it uses named components, it names its constraints after the specification, and it solves to `optimal`. It contains **exactly two defects**: one sign error and one missing constraint.

Specification. A plant calcines lithium iron phosphate cathode powder over five months. Let x_t be the tonnes produced in month t and I_t the tonnes in the warehouse at the end of month t.

- C1. Inventory balance: closing stock equals opening stock plus production minus shipments.
- C2. Nonnegativity: production and inventory are nonnegative; backorders are not allowed.
- C3. Kiln capacity: production in month t may not require more kiln hours than are available in month t, at 4.0 kiln hours per tonne.
- C4. Warehouse capacity: end-of-month stock may not exceed 60 t.
- C5. Closing safety stock: at least 15 t at the end of month 5.
- C6. Objective: minimize production cost plus inventory holding cost.

(a) Locate the sign error. Quote the offending line, state what the line says in words, and state what it should say.

(b) Locate the missing constraint. Name the specification item that is absent, and state the fingerprint in the listing that gives it away without running anything.

(c) For each defect separately, state the physical consequence: what the returned plan claims to do that a real plant could not do, and in which direction the reported cost is biased. Support each with one number taken from the printed output.

(d) Correct both defects and state the corrected optimal cost together with the corrected production and inventory plan. Report the difference between the reported cost of the defective model and the corrected optimum, in thousand baht and as a percentage of the corrected optimum.

Listing for Problem 6.

```
import pyomo.environ as pyo

PERIODS = [1, 2, 3, 4, 5]
demand  = {1:  80, 2: 120, 3: 160, 4: 140, 5: 100}     # t/month
kiln_h  = {1: 520, 2: 520, 3: 480, 4: 520, 5: 520}     # h/month
c_prod  = {1:1100, 2:1120, 3:1200, 4:1180, 5:1100}     # thousand baht/t
RATE    = 4.0     # kiln hours per tonne,        h/t
HOLD    = 25.0    # holding cost,   thousand baht/(t*month)
WAREH   = 60.0    # warehouse capacity,                   t
I_OPEN  = 20.0    # opening inventory,                    t
I_SAFE  = 15.0    # closing safety stock,                 t

m = pyo.ConcreteModel(name="lfp_plan")
m.T = pyo.Set(initialize=PERIODS, ordered=True)

m.d    = pyo.Param(m.T, initialize=demand)
m.H    = pyo.Param(m.T, initialize=kiln_h)
m.c    = pyo.Param(m.T, initialize=c_prod)
m.a    = pyo.Param(initialize=RATE)
m.h    = pyo.Param(initialize=HOLD)
m.W    = pyo.Param(initialize=WAREH)
m.I0   = pyo.Param(initialize=I_OPEN)
m.Imin = pyo.Param(initialize=I_SAFE)

m.x = pyo.Var(m.T, domain=pyo.NonNegativeReals)     # production, t
m.I = pyo.Var(m.T, domain=pyo.NonNegativeReals)     # end-of-month stock, t

def balance_rule(m, t):                             # C1
    prev = m.I0 if t == m.T.first() else m.I[t-1]
    return prev + m.x[t] - m.d[t] == m.I[t]
m.balance = pyo.Constraint(m.T, rule=balance_rule)

def warehouse_rule(m, t):                           # C4
    return m.I[t] <= m.W
m.warehouse = pyo.Constraint(m.T, rule=warehouse_rule)

m.safety = pyo.Constraint(expr=m.I[m.T.last()] >= m.Imin)          # C5

m.cost = pyo.Objective(                                             # C6
    expr=sum(m.c[t]*m.x[t] for t in m.T) - sum(m.h*m.I[t] for t in m.T),
```

```
    sense=pyo.minimize)

solver = pyo.SolverFactory("glpk")
res = solver.solve(m)
assert res.solver.termination_condition == pyo.TerminationCondition.optimal
print(f"reported total cost = {pyo.value(m.cost):,.1f} thousand baht")
for t in m.T:
    print(f"  month {t}: x = {pyo.value(m.x[t]):6.1f} t,"
          f" I = {pyo.value(m.I[t]):6.1f} t,"
          f" kiln = {RATE*pyo.value(m.x[t]):6.1f} h"
          f" (available {kiln_h[t]:.0f} h)")
```

Printed output of the listing.

```
reported total cost = 674,425.0 thousand baht
  month 1: x =  120.0 t, I =   60.0 t, kiln =  480.0 h (available 520 h)
  month 2: x =  120.0 t, I =   60.0 t, kiln =  480.0 h (available 520 h)
  month 3: x =  160.0 t, I =   60.0 t, kiln =  640.0 h (available 480 h)
  month 4: x =   80.0 t, I =    0.0 t, kiln =  320.0 h (available 520 h)
  month 5: x =  115.0 t, I =   15.0 t, kiln =  460.0 h (available 520 h)
```

Grading Rubric (Total: 100 points)

1. **Blending with quality specifications (20 pts)**
   - General formulation with all four constraint families and the model class (6)
   - Correct three-variable linear program in unnormalized form (4)
   - Elimination, solution, delivered conductivity and water content (8)
   - Active set and shadow-price statement (2)
2. **Ratio-constraint linearization (10 pts)**
   - General rule with the denominator condition (3)
   - Minimum-fraction constraint (2)
   - Stream-ratio constraint (1)
   - Two failure cases correctly classified (2)
   - Re-solved instance and the cost of the restriction (2)
3. **Pooling and nonconvexity (18 pts)**
   - Complete model with the bilinear terms identified (5)
   - Explanation of why multiplying through fails, with the correct balance named (3)
   - Both points verified feasible and the midpoint shown infeasible, with the conclusion

(5)

- Two fixed-p linear programs solved and the local-optimum conclusion (5)

4. **Big-M selection (16 pts)**
   - Fixed-charge constraint with all four tightest M_j derived (4)
   - Minimum operating level, with the statement that no M is needed (2)
   - Three logical conditions (4)
   - Either-or constraint with tightest M justified (3)
   - Three objective values, two gaps and the conclusion (3)

5. **Convex hull versus big-M (16 pts)**
   - Big-M formulation with all four tightest constants derived (5)
   - Convex hull formulation, correctly disaggregated (4)
   - Mixed-integer optimum with the selected technology (3)
   - Feasibility of the test point, its objective, and the separating valid inequality (4)

6. **Model audit (20 pts)**
   - Sign error located and stated in words (5)
   - Missing constraint located, with the fingerprint (5)
   - Physical consequence and direction of bias for each defect, each supported by a number (6)
   - Corrected optimum, corrected plan and the difference in baht and percent (4)

Reference. Rao, *Engineering Optimization: Theory and Practice*, 4th ed., Ch. 10; Williams, *Model Building in Mathematical Programming*, Ch. 9; Biegler, *Nonlinear Programming*, Ch. 1.