Introduction to Optimization Modeling

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PETRONAS Data Science Department, KLCC Tower 3

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Agenda

Time	Day 1	Day 2
9:00–10:00	PART 1: Introduction—Background and Applications	PART 3: Introduction to Discrete Optimization (MILP, MINLP)
10:00–10:30	Working Session 1: Refinery planning (LP)	Working Session 3: Asset inventory (MILP)
10:30–11:00	Morning Break	Morning Break
11:00–12:00	Working Session 1 (practice)	Working Session 3 (practice)
12:00–1:00	Working Session 1 (solution)	Working Session 3 (solution)
1:00–2:00	Lunch	Lunch
2:00–2:30	PART 2: Introduction to Continuous Optimization (LP, NLP)	Working Session 4: Gasfield planning (MINLP)
2:30–3:30	Working Session 1 (extension)	Working Session 4 (practice)
3:30–4:00	Afternoon Break	Afternoon Break
4:00–4:30	Working Session 2: Compressor (NLP)	Working Session 4 (solution)
4:15–4:45	Working Session 2 (solution)	Conclusion
4:45–5:00	Day 1 review and Day 2 overview	Wrap up and next steps

About myself

- Senior lecturer, Chemical Engineering Department, UTP
- Consultant/Engineer, Kuala Lumpur (2014–2017)
  - Develop, deploy, & sustain process operation models for refineries & petrochemicals
- PhD in Chemical Engineering, Imperial College, UK (2010–2013)
  - Specialization: Process systems engineering
  - Thesis: Modeling & optimization of industrial water systems
- Masters of Applied Science in Chemical Engineering, University of Waterloo, Ontario, Canada (2005–2007)
  - Specialization: Systems design engineering
  - Thesis: Petroleum refinery planning under uncertainty
- Representative publications:

Albahri, TA, **CS Khor,** M Elsholkami, A Elkamel (2019). A mixed integer nonlinear programming approach for petroleum refinery topology optimisation. *Chemical Engineering Research & Design* 143: 24-35.

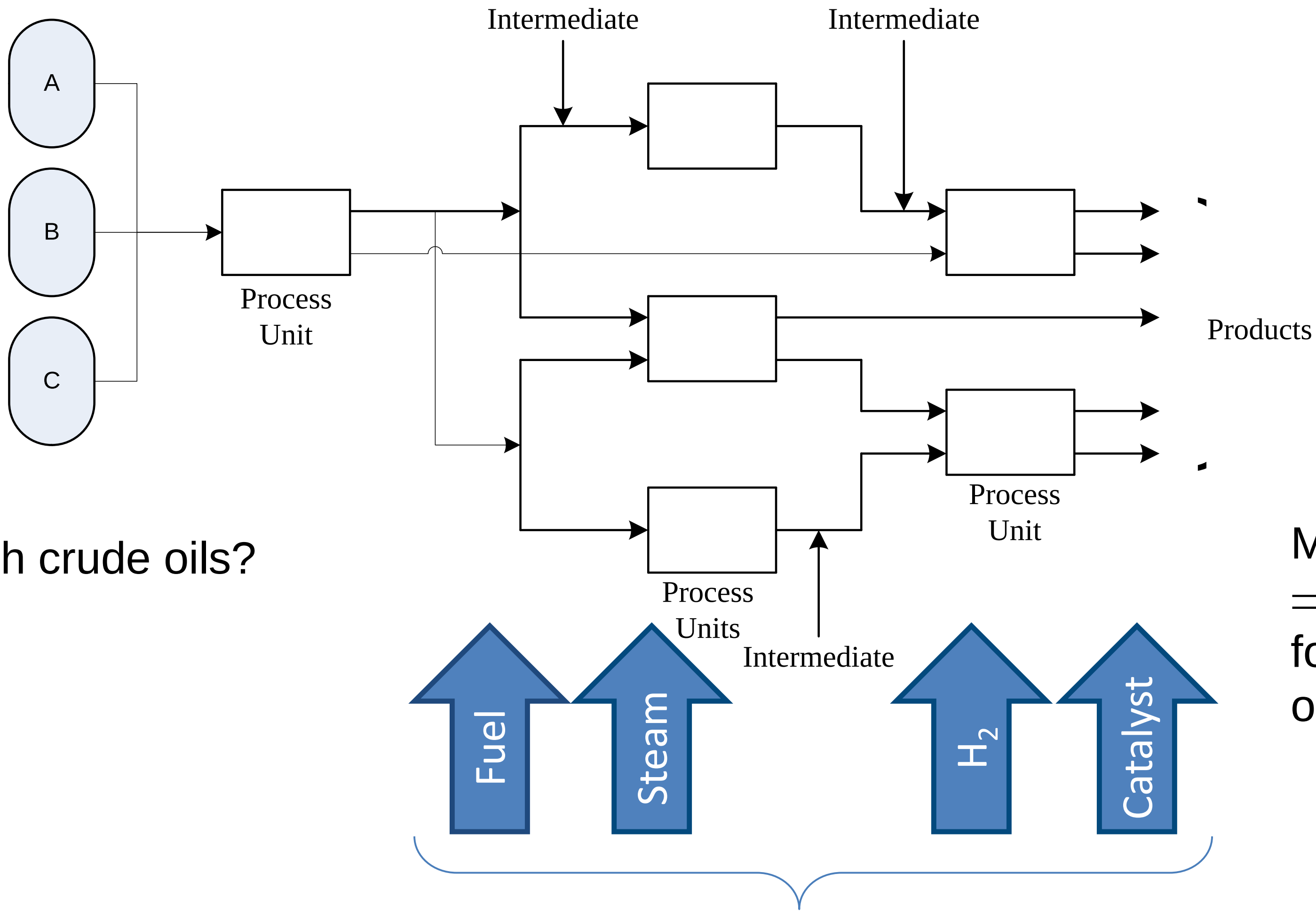
Khor, CS, B Chachuat, N Shah (2012). A superstructure optimization approach for water network synthesis with membrane separation-based regenerators. *Computers & Chemical Engineering* 42: 48–63.

Khor, CS, A Elkamel, K Ponnambalam, PL Douglas (2008). Two-stage stochastic programming with fixed recourse via scenario planning with economic and operational risk management for petroleum refinery planning under uncertainty. *Chemical Engineering & Processing* 47 (9–10): 1744–1764

Course objectives

1. Identify decision variables based on problem description.
2. Formulate constraints based on data available or needed.
3. Formulate objective function (maximization or minimization) based on data and constraints.
4. Determine optimization model type to choose suitable solution method.
5. Interpret solution in terms of physical meaning and significance

Working Session 1
Refinery planning (LP)



Which products?

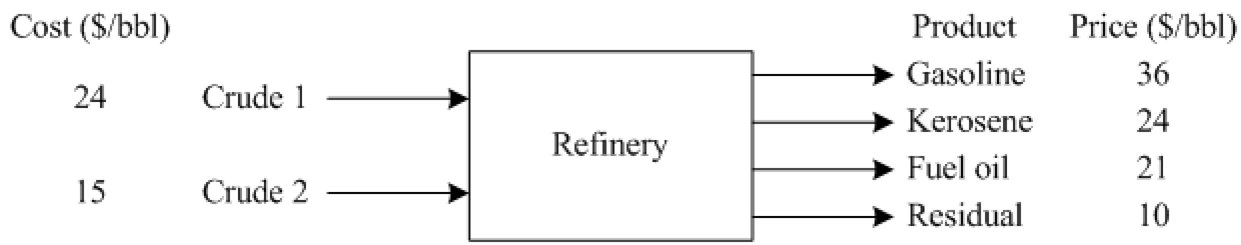
Which crude oils?

Margins usually low
⇒ strong incentive for refiners to optimize operations

Less utilities?

Working Session 1
Refinery planning

Task: A schematic of a simple refinery (topping) is shown. Formulate a model to maximize the refinery profit. Explain how you can solve the model (by hand/manually). Then check the solution using Excel Solver.



	Volume percent yield		Maximum allowable production (bbl/day)
	Crude 1	Crude 2	
Gasoline	80	44	24,000
Kerosene	5	10	2,000
Fuel oil	10	36	6,000
Residual	5	10	–
Processing cost ($/bbl)	0.5	1	–

Working Session 1
Refinery planning (LP): Solution

maximize Profit = $8.1x_1 + 10.8x_2$

LP1: $0.8x_1 + 0.44x_2 \leq 24000$

LP2: $0.05x_1 + 0.1x_2 \leq 2000$

LP3: $0.1x_1 + 0.36x_2 \leq 6000$

LP4: $x_1 \geq 0$

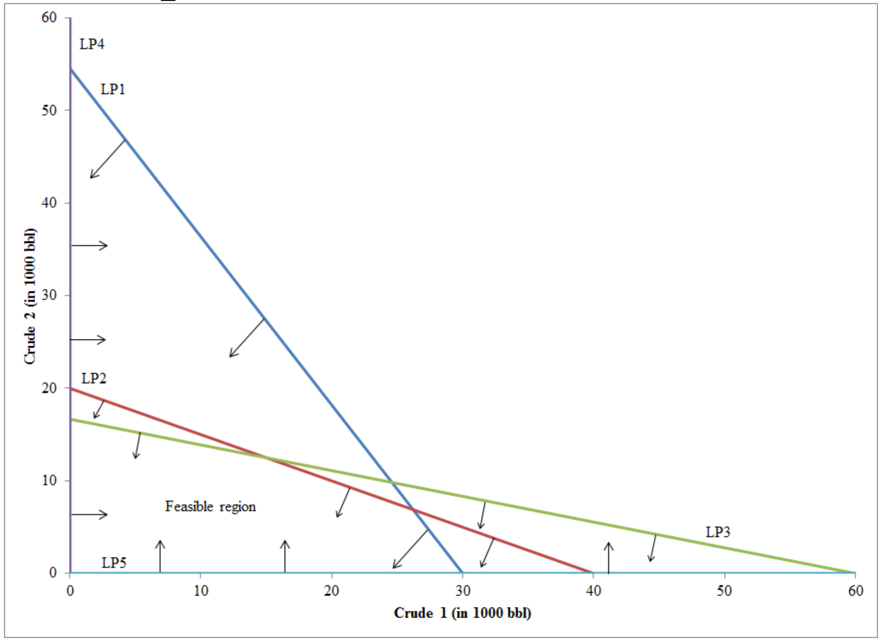
LP5: $x_2 \geq 0$

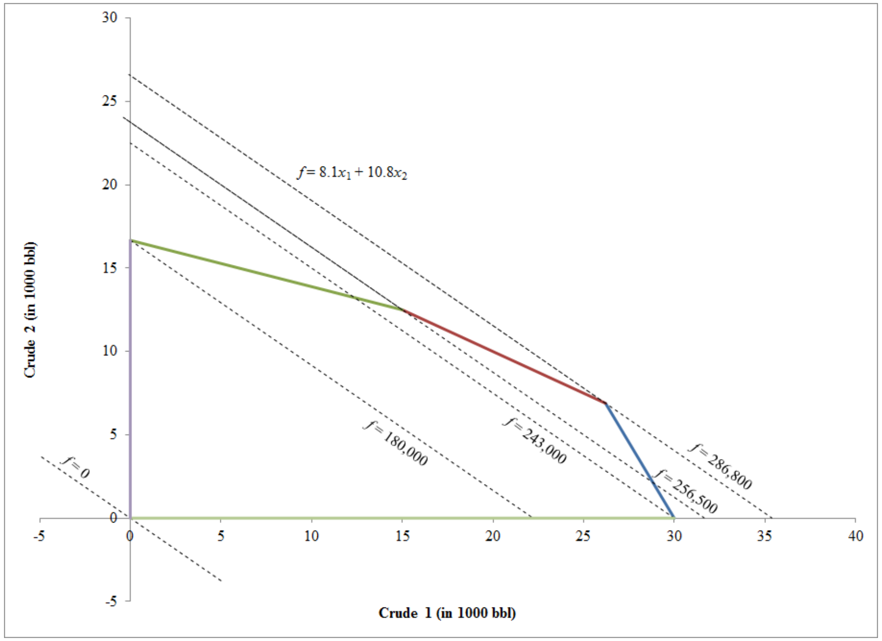
Optimal solution:

$x_1^* = 26{,}000$ bbl/day

$x_2^* = 7{,}000$ bbl/day

$f(x^*) = 286{,}800$ \$/day





Working Session 1 (Homework)

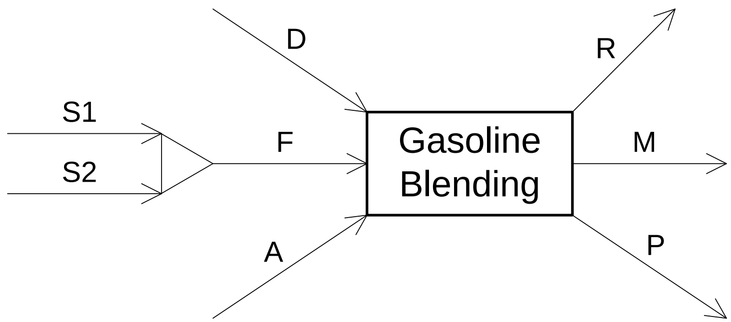
Refinery planning (LP)

Homework: You are working in the process planning department of a refinery. You are asked to produce a minimum 1.5 MMgal/day of gasoline, minimum 2 MMgal/day of diesel, and minimum 1 MMgal/day of kerosene. (MM stands for million.) Table shows how much gasoline, diesel, and kerosene are produced from each crude. Determine the optimal crude oil types to use (which and how much) with an appropriate economic objective (use Excel Solver with sensitivity report).

Crude Oil Type	Cost (USD/bbl)	Gasoline (gal/bbl)	Diesel (gal/bbl)	Kerosene (gal/bbl)
A	50	10	20	15
B	80	15	15	20
C	100	20	10	15

Solution: $x_A^* = 8.33\text{E}+04$ bbl, $x_C^* = 3.33\text{E}+04$ bbl, $f(x^*) = 7.50$ million USD/day

Working Session 1 (extension)
Refinery blending



Tasks: Formulate a nonlinear gasoline blending model for the pooling problem. Solve the model using Excel Solver (will try GAMS later).

Component (Feedstock) Characteristics			
Component	RON	Cost ($/gal)	Availability ('000 gal/mo)
Domestic Blend	85	0.65	10,000
Foreign Blend			8,000
Source 1	93	0.80	
Source 2	97	0.90	
Premium Additive	900	30	50

Product Characteristics			
	Minimum RON	Sales Price ($/gal)	Minimum Demand ('000 gal/mo)
Regular Unleaded	87	1.18	100
Midgrade Unleaded	89	1.25	100,000
Premium Unleaded	94	1.40	100,000

Working Session 1 (extension)
Refinery blending: Solution

- Formulation (NLP):

$$
\begin{aligned}
\min \quad & 1.18R + 1.25M + 1.40P \\
\text{s.t.} \quad & R = RD + RF \\
& M = MD + MF \\
& P = PD + PF + A \\
& D = RD + MD + PD \\
& RF + MF + PF = S1 + S2 \\
& 85RD + xRF \geq 87R \\
& 85MD + xMF \geq 89M \\
& 85PD + xPF + 900A \geq 94P \\
& x(S1 + S2) = 93S1 + 97S2 \\
& S1 + S2 \leq 8000 \\
& D \leq 10000 \\
& A \leq 50 \\
& R, M, P \geq 100 \\
& \forall \text{variables} \geq 0
\end{aligned}
$$

- *Bonus*: Can we formulate an (equivalent) LP for this problem?

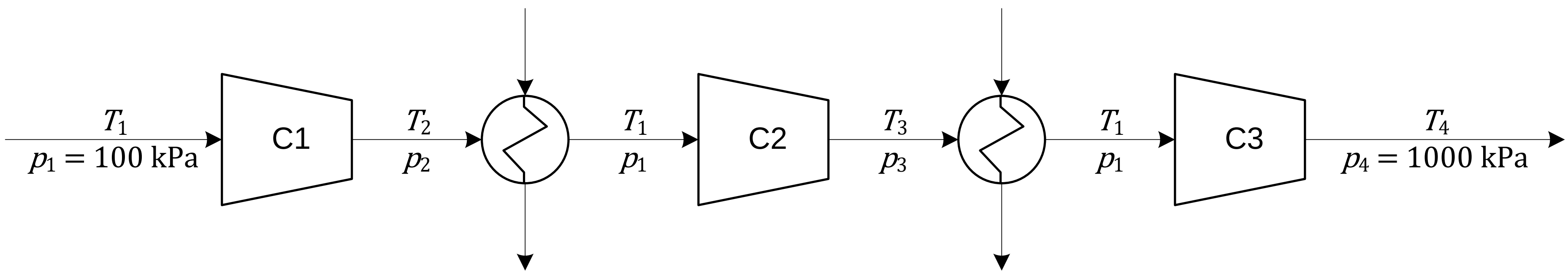
Working Session 2
Compressor operation (NLP)

Consider compression work for ideal compressible adiabatic flow. The relation between gas pressure and density cannot be established because temperature is unknown as function of pressure or density, hence it is derived using mechanical energy balance.

- Theoretical compression work per mol (or mass) of gas:

(1 stage)

$$\widehat{W}_1 = \frac{k}{k-1} R T_{\text{in}} \left[\left(\frac{p_2}{p_1} \right)^{(k-1)/k} - 1 \right]$$



Working Session 2
Compressor operation

Task: For a 3-stage compressor with intercooling back to suction temperature (T_{in}) in between stages, determine the optimal interstage pressures p_2 and p_3 to minimize $\widehat{W}$ keeping p_1 (100 kPa) and p_4 (1000 kPa) fixed. Solve the model using Excel Solver. [*Bonus*: Compare/Check the solution using an analytical approach (by hand).]

- Assumptions:

  Ideal gas $\Rightarrow pV^k$ = constant

  Constant $k = C_p / C_v$ = 1.4 (air)

  R = 8.3145 J/(k·mol)

- Objective function: minimize compression work

(3 stages) $$\widehat{W}_3 = \frac{k}{k-1} R T_{\text{in}} \left[\left(\frac{p_2}{p_1}\right)^{(k-1)/k} + \left(\frac{p_3}{p_2}\right)^{(k-1)/k} + \left(\frac{p_4}{p_3}\right)^{(k-1)/k} - 3 \right]$$

Working Session 2
Solution

- Decision variables: p_2, p_3, T_{in} (V?)

$$\min \quad \widehat{W}_3 = \frac{k}{k-1} R T_{\text{in}} \left[\left(\frac{p_2}{p_1}\right)^{(k-1)/k} + \left(\frac{p_3}{p_2}\right)^{(k-1)/k} + \left(\frac{p_4}{p_3}\right)^{(k-1)/k} - 3 \right]$$

$$\text{s.t.} \quad \frac{T_{\text{in}}}{V^k} = \frac{p_{\text{in}}}{R}$$

Working Session 3
Downstream asset inventory management (MILP)

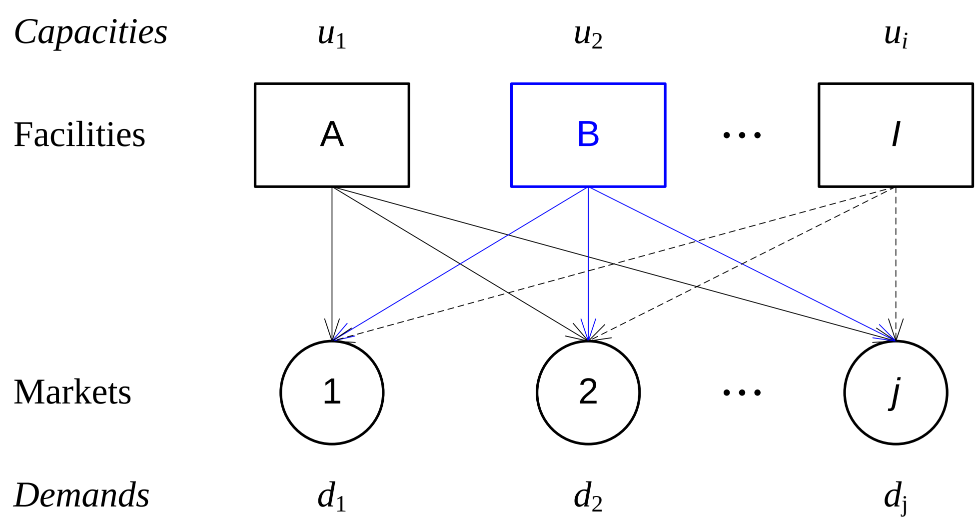
- General formulation for transportation (LP)/facility location problem (MILP):

LP

$$\begin{aligned} \min \quad & \textstyle\sum_i \sum_j c_{ij} x_{ij} \\ \text{s.t.} \quad & \textstyle\sum_j x_{ij} \le a_i\,, \quad \forall i \\ & \textstyle\sum_i x_{ij} \ge b_j\,, \quad \forall j \\ & x_{ij} \ge 0, \quad \forall i,j \end{aligned}$$

MILP

$$\begin{aligned} \min \quad & \textstyle\sum_i \sum_j c_{ij} x_{ij} + \sum_i f_i y_i & \text{(fixed charge)} \\ \text{s.t.} \quad & \textstyle\sum_j x_{ij} \le u_i y_i\,, \quad \forall i & \text{(supply limit)} \\ & \textstyle\sum_i x_{ij} \ge b_j\,, \quad \forall j & \text{(demand requirement)} \\ & x_{ij} \ge 0, \quad \forall i,j & \text{(non-negativity)} \\ & y_i = 0 \text{ or } 1, \quad \forall i,j & \text{(integrality)} \end{aligned}$$



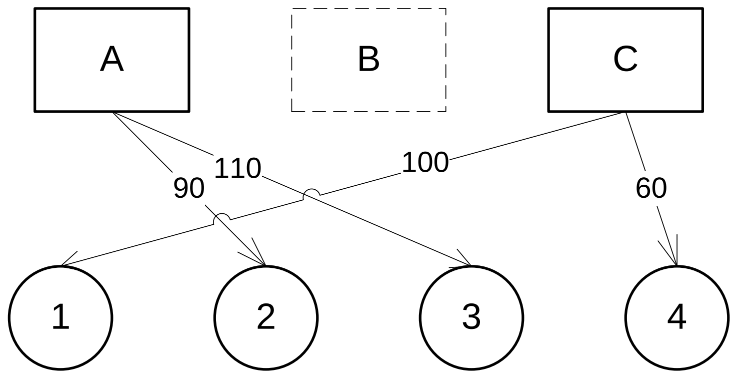
Working Session 3
Downstream asset inventory management

Task: (warehouse location problem) A steel wholesaler leases its regional warehouses to conserve capital. 3 warehouses can be leased at a monthly cost. Each warehouse can load a maximum number of trucks per month as in given data. Determine which warehouses to lease and how many trucks to send from each warehouse to each district. Solve the model using Excel (and later GAMS).

	Cost/Truck ($)					
Warehouse	District 1	District 2	District 3	District 4	Monthly Capacity (no. of trucks)	Monthly Leasing Cost ($)
A	170	40	70	160	200	7750
B	150	195	100	10	250	4000
C	100	240	140	60	300	5500
Monthly Demand	100	90	110	60		

Working Session 3
Solution

- Variables:
  - warehouse selection (binary 0–1)
  - number of trucks (continuous or integer?)



Working Session 3 (extension)
Transportation problem (using GAMS)

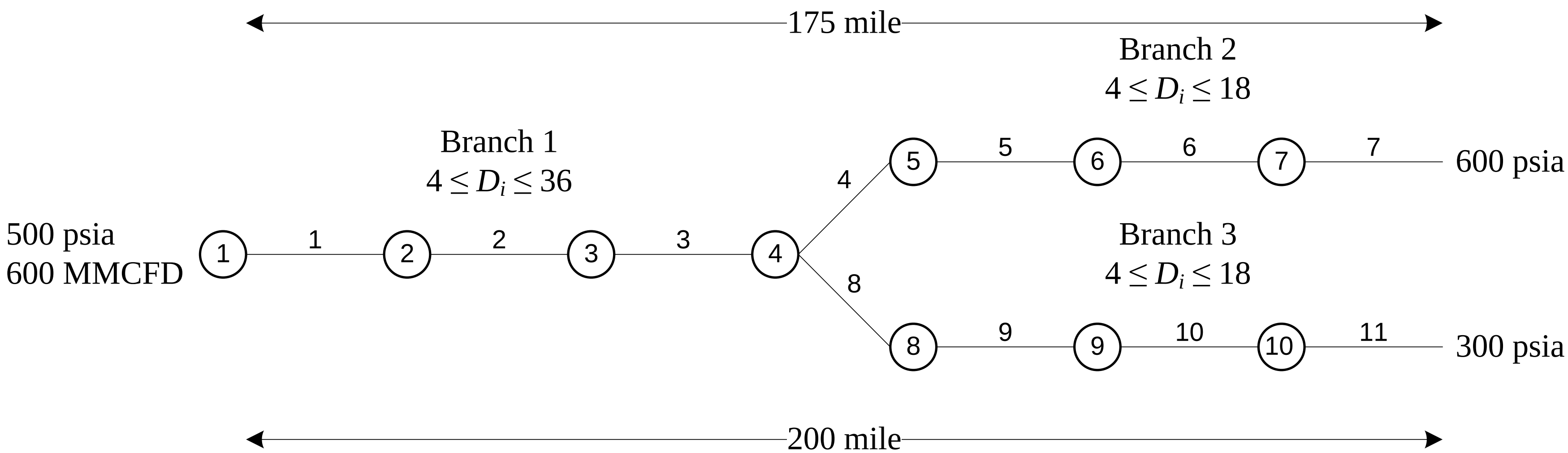
Task: Consider 2 plants and 3 markets as given in the table. Assume shipping costs to be $90.00 per case per thousand miles. Determine the optimal shipment between plants and markets to minimize total transport cost.

Shipping Distance (mile)

	Market			Supply (case)
	New York	Chicago	Topeka	
Seattle	2.5	1.7	1.8	350
San Diego	2.5	1.8	1.4	600
Demand	325	300	275	

Working Session 4
Upstream gasfield planning (NLP, MINLP)

Gas gathering and transmission system consists of sources of gas (from wells in reservoir), pipelines, compressor stations, and delivery (demand) sites. Design or expansion planning of gas pipeline transmission involves fixed capital cost as well as variable operating and maintenance cost.



Working Session 4
Upstream gasfield planning (NLP, MINLP)

Task: Determine an optimal gas transmission system for the given configuration of one gas well and two demand points to transport a prespecified gas quantity per time.

- Variables: length (mile) L_i, discharge pressure (psi) pd_i, suction pressure (psi) ps_i, diameter (in.) D_i, flow rate (MMCFD) Q_i, compression ratio cr_j, work W_j
- Cost data: c_c = compressor capital cost (10,000 \$/(hp·year)), c_o = annual operating cost (70.00 \$/(hp·year)), c_i = pipe capital cost (\$870/(in.·mile·year))

min $\quad \sum_j (c_c + c_o) W_j + \sum_i c_i L_i D_i$

s.t. $\quad ps_i \le pd_i \le \mathrm{cr}_j ps_{i-1}$ (line pressure drop)

$pd_i = \mathrm{cr}_j ps_{i-1}$ (compression ratio)

$(871 \times 10^{-6})^2 D_i^{(16/3)} \left(pd_i^2 - ps_i^2\right) - L_i Q_i^2 = 0$ (flow definition)

$W_j = (0.08531) Q_i \frac{k}{k-1} T_{\mathrm{in}} \left[\left(\frac{pd_i}{ps_{i-1}} \right)^{z(k-1)/k} - 1 \right]$ (compression work)

$\sum_{i=1}^{3} L_i + \sum_{i=4}^{7} L_i = 175, \sum_{i=1}^{3} L_i + \sum_{i=8}^{11} L_i = 175$ (line length)

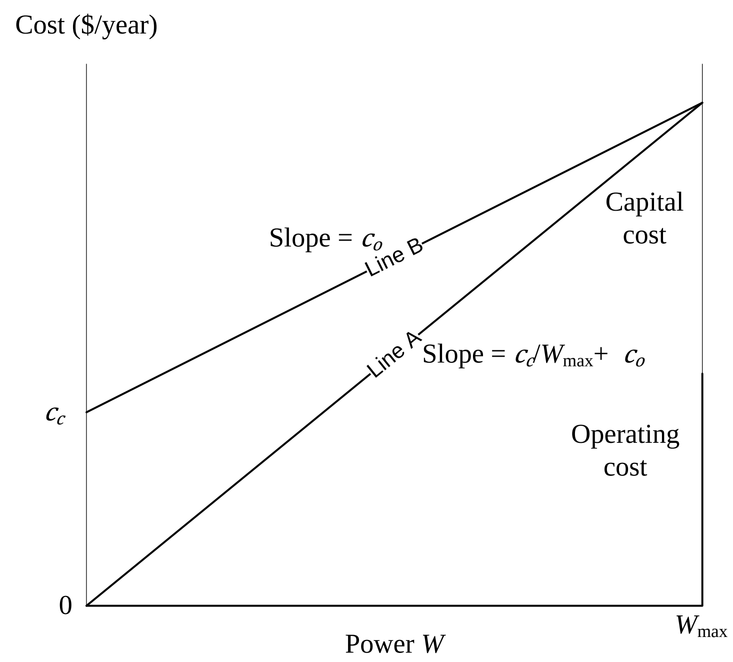
$\mathrm{cr}_j \le \left(\mathrm{cr}_j^{\mathrm{U}} - 1\right) y_j + 1$ (compressor selection)

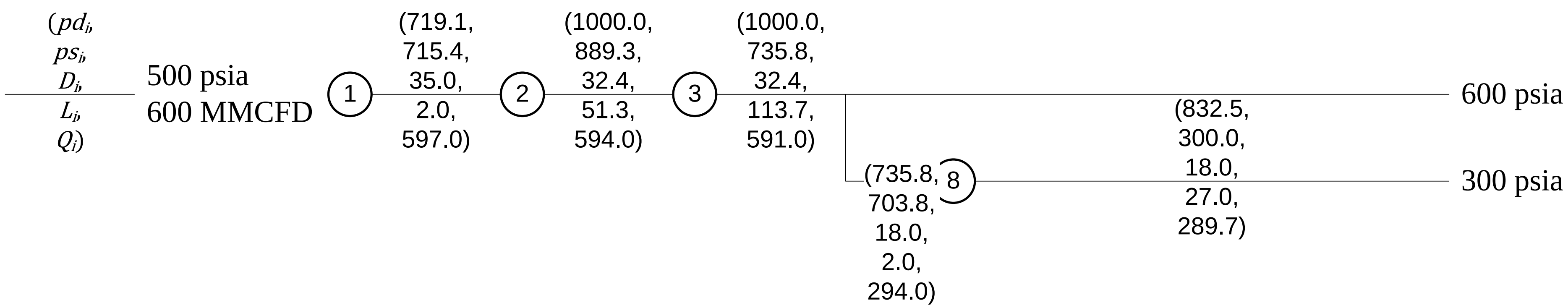
$200 \le pd_i \le 1000,\ 200 \le ps_i \le 1000$ (simple bounds)

$2 \le L_i \le 200,\ 1 \le \mathrm{cr}_j \le 2,\ 200 \le Q_i \le 600$

$W_j \ge 0$ (non-negativity)

Working Session 4
Solution





Concluding remarks

- LP/MILP:
  - minimization (maximization) objective usually has “$\geq$” (“$\leq$”) constraint
  - standard formulations available
  - can handle large problems (constraints and variables)
  - useful solution interpretation (sensitivity analysis)

- NLP/MINLP:
  - initial values important for solution (speed, global optimality)
  - choose/tailor solution method to problem structure
  - consider reformulating (linearized) to converge or reduce time (solution may be comparable/acceptable)
  - sensitivity analysis less well developed

References

Working session problems:

Edgar, T.F., D.M. Himmelblau, L.S. Lasdon. *Optimization of Chemical Processes*. McGraw-Hill, 2001.

Eppen, G. D., F. J. Gould, C. P. Schmidt, J. H. Moore, L. R. Weatherfood. *Introductory Management Science*. 5th ed. Prentice-Hall, 1998.

GAMS: A User's Guide.

Textbooks:

William, H. P. *Model Building in Mathematical Programming*. Wiley, 1978.

- Accessible text on good practices to formulate LP/ILP/MILP models

Rardin, R. L. *Optimization in Operations Research*. New Jersey: Prentice-Hall, 1998.

- Clearly-written text on models and algorithms covering both continuous and discrete optimization

Other references:

Avriel, M, B. Golany (eds). *Mathematical Programming for Industrial Engineers*. Dekker, 1996.

Nemhauser, G.L., L.A. Wolsey. *Integer and Combinatorial Optimization*. Wiley 1988.

- Readable mathematical treatment of various practical optimization aspects in model formulation and solution

Biegler, L.T., I.E. Grossmann, A//W. Westerberg. *Systematic Methods of Chemical Process Design*. Prentice Hall, 1997.

– Covers both models and solution strategies for mixed-integer problems in process systems engineering

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Thank You

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