CHN-323
Computer Applications in Chemical Engineering

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Example 1

An object is being projected upward at a specified velocity. It is subject to linear drag and its altitude as a function of time can be computed as

$$z = z_0 + \frac{m}{c}\left(v_0 + \frac{mg}{c}\right)\left(1 - e^{-(c/m)t}\right) - \frac{mg}{c}t$$

where

z = altitude (m) above the earth's surface (defined as z = 0)

t = time (s)

z_0 = the initial altitude (m) =100 m

m = mass (kg) =80 kg

c = a linear drag coefficient (kg/s) = 15 kg/s

v_0 = initial velocity (m/s)=55 m/s

Plot z vs t till the object returns to the ground.

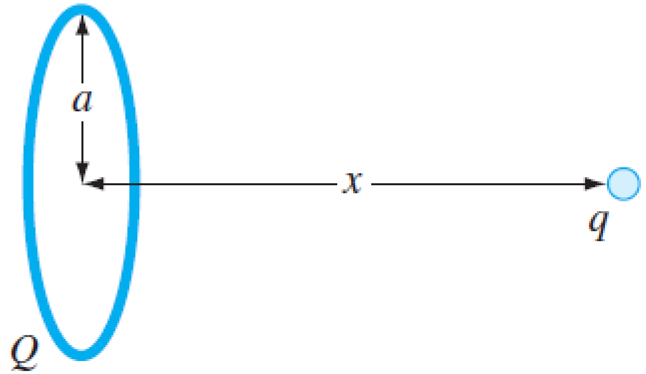
Find the time at which the maximum elevation is achieved?

- With the graph
- With optimization principles

Example 2

A total charge Q is uniformly distributed around a ring-shaped conductor with radius *a*. A charge *q* is located at a distance *x* from the center of the ring. The force exerted on the charge by the ring is given by

$$F = \frac{1}{4\pi e_0} \frac{qQx}{(x^2 + a^2)^{3/2}}$$



where $e_0 = 8.85 \times 10^{-12}\ C^2/(N.m^2)$, $q = Q = 2 \times 10^{-5}\ C$, and $a = 0.9$ m.

Determine the distance *x* where the force is a maximum.

Example 3

A train (series) of four well mixed reactors operate isothermally. The species whose concentration is designated by c reacts according to the mechanism: $r = -kc^n$ in each tank. The fluid flow rate is at a fixed value q. Each tank has a volume V_i (i = 1, ..., 4).

The material balance for any reactor i is written as

$$\frac{d(V_i\, c_i)}{dt} = q\, c_{i-1} - q\, c_i - V_i\, k\, c_i^n$$

Determine the volume of each reactor such that the *steady state* yield of the product is maximum. The total volume of the four tanks is 20 m^3. The values of the parameters and operating variables are n = 2.5, q = 71 m^3/h, inlet concentration into first reactor c_0 = 20 kg mol/m^3 and k = 6.25×10^{-3} $[m^3/\text{kg mol}]^{1.5}(s)^{-1}$.

Minimize: outlet reactant concentration (or maximize product concentration)

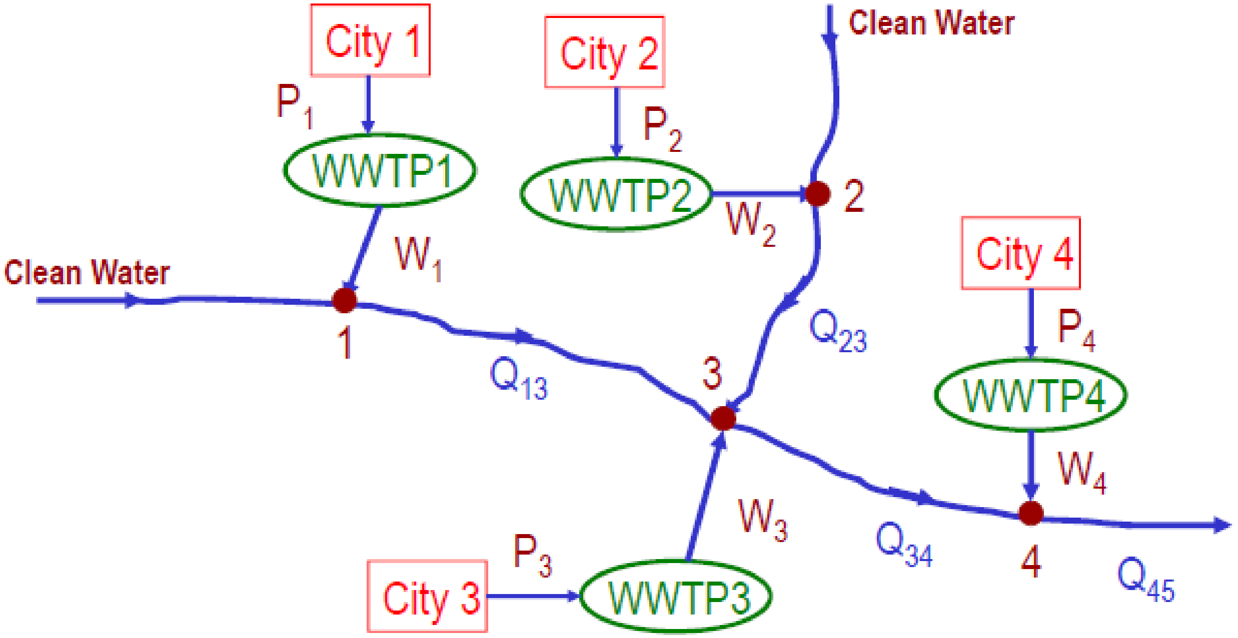
w.r.t v_i, i=1,..,4

Bounds: $v_i > 0$

Constraints: $\sum v_i = 20$

Example 3

Minimize the cost of waste-water treatment in a city consortium while maintaining the pollutant concentration in any stream not greater than 20 mg/L.



WWTP – Waste Water Treatment Plant
P_i = waste generated by City i (mg / day); i = 1, 2, 3, 4
W_i = waste discharged by City i (mg / day); i = 1, 2, 3, 4
x_i = fraction waste removed by WWTPi; i = 1, 2, 3, 4
c_i = concentration of pollutant at junction i (mg / L); i = 1, 2, 3, 4
Q_{ij} = Vol. flow rate between junction i and junction j (L / day)
R_{ij} = fraction of pollution remaining as the river flows downstream from junction i to junction j (pollutant level is reduced due to chemical & biological decomposition processes)
d_i = cost of waste treatment in WWTPi ($/mg)

City	P_i (mg/day)	d_i ($\$10^{-6}$/mg)	Segment	Q (L/day)	R
1	1×10^9	2	1-3	1×10^7	0.5
2	2×10^9	2	2-3	5×10^7	0.35
3	4×10^9	4	3-4	11×10^7	0.6
4	2.5×10^9	4	4-5	25×10^7	

Solution

Total cost of wastewater treatment in a day

Cost = $d_1 P_1 x_1 + d_2 P_2 x_2 + d_3 P_3 x_3 + d_4 P_4 x_4$

Pollutant concentrations at every junction

$$c_1 = \frac{(1 - x_1)P_1}{Q_{13}}$$

$$c_2 = \frac{(1 - x_2)P_2}{Q_{23}}$$

$$c_3 = \frac{Q_{13}R_{13}c_1 + Q_{23}R_{23}c_2 + (1 - x_3)P_3}{Q_{34}}$$

$$c_4 = \frac{Q_{34}R_{34}c_3 + (1 - x_4)P_4}{Q_{45}}$$

Example: fmincon

- $f(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$ **Rosenbrock function**

- Find the minimum value starting from the point [-1,2], constrained to have $x_1 + 2x_2 \leq 1$.
- Express this constraint in the form *Ax* <= b by taking *A* = [1,2] and b = 1.
- Notice that this constraint means that the solution will not be at the unconstrained solution (1,1), because at that point $x_1 + 2x_2 = 3 > 1$.

- fun = @(x)100*(x(2)-x(1)^2)^2 + (1-x(1))^2;

- x0 = [-1,2];
- A = [1,2];
- b = 1;
- x = fmincon(fun,x0,A,b)

- $f(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$

- Find the minimum value starting from the point [0.5,0], constrained to have $x_1 + 2x_2 \leq 1$ and $2x_1 + x_2 = 1$.

- Express the linear inequality constraint in the form *A**x <= b by taking *A* = [1,2] and b = 1.

- Express the linear equality constraint in the form

*Aeq**x = beq by taking *Aeq* = [2,1] and beq = 1.

```
fun = @(x)100*(x(2)-x(1)^2)^2 + (1-x(1))^2;
x0 = [0.5,0];
A = [1,2];
b = 1;
Aeq = [2,1];
beq = 1;
x = fmincon(fun,x0,A,b,Aeq,beq)
```