IIT KHARAGPUR

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CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Applications of Optimization

(WEEK – 11: LECTURE – 51)

Dr. Debasis Sarkar

Department of Chemical Engineering

Indian Institute of Technology Kharagpur

Applications of Optimization

Week 11:

- Optimization of various chemical and biochemical processes

MATLAB Function `fmincon`

MATLAB function `fmincon` solves a General Nonlinear Programming Problem as follows:

$$\underset{x}{\text{Minimize}} \quad f(x)$$

$$\text{Such that:} \quad c(x) \le 0$$

$$c_{eq}(x) = 0$$

$$A \cdot x \le b$$

$$A_{eq} x = b_{eq}$$

$$LB \le x \le UB$$

MATLAB Function fmincon : Syntax

```
x = fmincon(fun,x0,A,b)
x = fmincon(fun,x0,A,b,Aeq,beq)
x = fmincon(fun,x0,A,b,Aeq,beq,lb,ub)
x = fmincon(fun,x0,A,b,Aeq,beq,lb,ub,nonlcon)
x = fmincon(fun,x0,A,b,Aeq,beq,lb,ub,nonlcon,options)
```

```
[x,fval] = fmincon(___)
[x,fval,exitflag,output] = fmincon(___)
[x,fval,exitflag,output,lambda,grad,hessian] = fmincon(___)
```

More information at:

https://in.mathworks.com/help/optim/ug/fmincon.html

MATLAB Function fmincon : Example

Minimize $f(x, y) = x + y$

Subject to: $x^2 + y^2 = 1$

```
function f = func(X)
        x = X(1);
        y = X(2);
        f = x + y;
end
```

```
function [c,ceq] = nonlincon(X)

% function for the nonlinear constraints.
% We have to define two outputs for fmincon: the
% nonlinear inequality contraints, and the equality
% constraints.
% C(X) <= 0
% Ceq(X) = 0

        x = X(1);
        y = X(2);
        c = [];
        ceq = x^2 + y^2 - 1;
end
```

MATLAB Function fmincon : Example

```
A   =  [];
B   =  [];     % the linear inequality constraints: A*X <= B
Aeq =  [];
Beq =  [];     % the linear equality constraints: Aeq*X = B
LB  =  [];
UB  =  [];     % LB <= X <= UB
X0  =  [1, 1]; % initial guess

[X,FVAL,EXITFLAG,OUTPUT,LAMBDA] = fmincon(@func,X0,A,B,Aeq,Beq,LB,UB,@nonlincon)
```

MATLAB Function fmincon : Example

```
X =
    0.7071    0.7071
FVAL =
    1.4142
EXITFLAG =
     5


LAMBDA =

         lower: [2x1 double]
         upper: [2x1 double]
         eqlin: [1x0 double]
       eqnonlin: 0.7071
        ineqlin: [1x0 double]
     ineqnonlin: [1x0 double]
```

```
OUTPUT =
iterations: 5
          funcCount: 15
       lssteplength: 1
           stepsize: 5.9440e-05
          algorithm: 'medium-scale: SQP,
Quasi-Newton, line-search'
      firstorderopt: 7.9553e-06
    constrviolation: 2.3986e-11
            message: [1x772 char]
```

MATLAB Function `fsolve`

The MATLAB function `fsolve` solves a system of nonlinear equations as represented by:

$$f(x) = 0$$

for x, where $f(x)$ is a function that returns a vector value. x is a vector or a matrix.

Syntax:

```
x = fsolve(fun,x0)
x = fsolve(fun,x0,options)

[x,fval,exitflag,output] = fsolve(___)
[x,fval,exitflag,output,jacobian] = fsolve(___)
```

`fsolve` is a part of MATLAB Optimization Toolbox.

`fsolve` starts at x0 and tries to solve the equations described in `fun`.

Algorithm: Choose between 'trust-region-dogleg' (default), 'trust-region', and 'levenberg-marquardt'.

MATLAB Function `fsolve` : Example

Solve:

$$2x_1 - x_2 = e^{-x_1}$$

$$-x_1 + 2x_2 = e^{-x_2}$$

starting at x0 = [-5 -5].

First, write an M-file that computes f, the values of the equations at x.

```
function f = myfun(x)
f(1) = 2*x(1) - x(2) - exp(-x(1));
f(2) = -x(1) + 2*x(2) - exp(-x(2))];
```

Next, call the optimization routine.

```
x0 = [-5; -5]; % Make a starting guess at the solution
options = optimset('Display','iter'); % Option to display output
[x,fval] = fsolve(@myfun,x0,options)  % Call optimizer
```

More information at: https://in.mathworks.com/help/optim/ug/fsolve.html

MATLAB Function `fsolve` : Example

Solve:

$$2x_1 - x_2 = e^{-x_1}$$

$$-x_1 + 2x_2 = e^{-x_2}$$

starting at x0 = [-5 -5].

```
x =
        0.5671
        0.5671

fval = 1.0e-008 *
          -0.5320
          -0.5320

Optimization terminated successfully.
```

Example

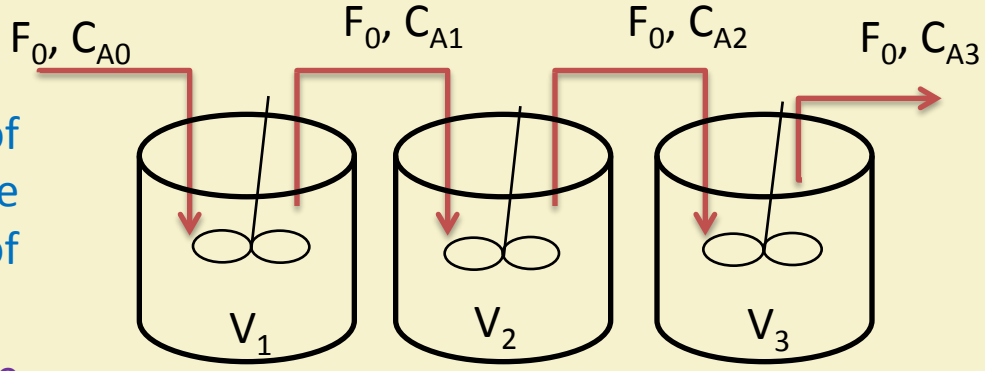
Continuous Stirred Tank Reactors (CSTR) in Series:

What should be the volume of each reactor so that the conversion of a reactant is maximized?

Reactors in Series

Three Continuous Stirred Tank Reactors (CSTRs) are connected in series. In these reactors, a reaction that consumes component A takes place: A → Product

The volumetric flow rate to each CSTR is same (F_0).

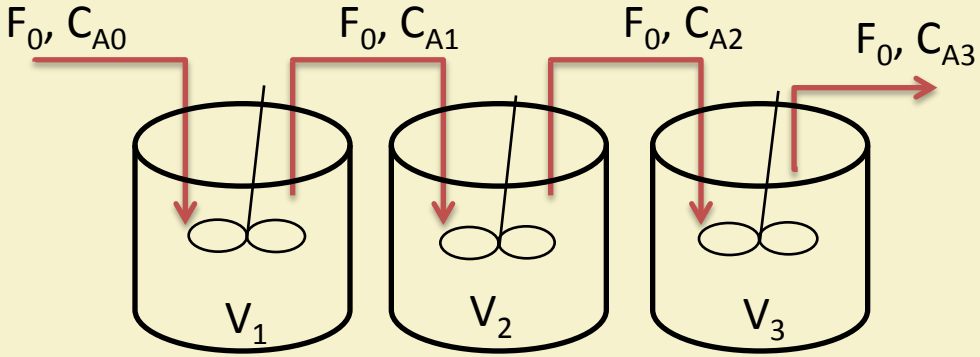


The objective is to determine the volumes of Reactors 1, 2, and 3 that minimize the concentration of reactant (A) at the outlet of the third reactor (C_{A3}).

There is a constraint that the total volume (i.e., the sum of the volumes of all three reactors) must be less than or equal to 7 m^3.

Reaction constant k = 1.0 $m^{1.5}/(hr\ kmol^{0.5})$
Volumetric flow rate F_0 = 2.0 m^3/hr
Feed concentration of reactant A, C_{A0} = 1 $kmol/m^3$

Reactors in Series: Modeling



A → Product

Mass Balances:

$$F_0\left(C_{A(i-1)} - C_{Ai}\right) = r_{Ai}V_i, \quad i \in \{1,2,3\}$$

Reaction Rates:

$$r_{Ai} = kC_{Ai}^{1.5}, \quad i \in \{1,2,3\}$$

Mass Balances:

$$2(C_{A0} - C_{A1}) = r_{A1}V_1$$
$$2(C_{A1} - C_{A2}) = r_{A2}V_2$$
$$2(C_{A2} - C_{A3}) = r_{A3}V_3$$

Reaction Rates:

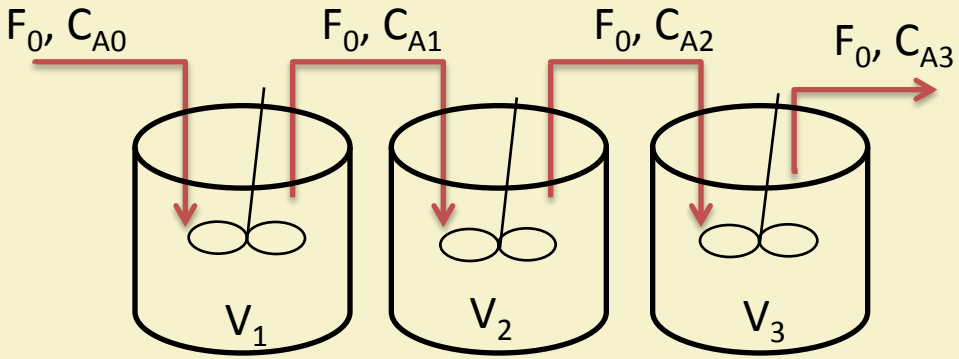
$$r_{A1} = C_{A1}^{1.5}$$
$$r_{A2} = C_{A2}^{1.5}$$
$$r_{A3} = C_{A3}^{1.5}$$

Reaction constant k = 1.0 $m^{1.5}/(hr\ kmol^{0.5})$

Volumetric flow rate F_0 = 2.0 m^3/hr

Feed concentration of reactant A, C_{A0} = 1 $kmol/m^3$

Reactors in Series: Problem Formulation



A → Product

Mass Balance

$$F_0\left(C_{A(i-1)} - C_{Ai}\right) = r_{Ai}V_i, \quad i \in \{1,2,3\}$$

Reaction Rate

$$r_{Ai} = kC_{Ai}^{1.5}, \quad i \in \{1,2,3\}$$

Find CSTR volumes to minimize C_{A3}.

$$\underset{V}{\text{minimize}}\ C_{A3}$$

Subject to

$$2(C_{A0} - C_{A1}) - r_{A1}V_1 = 0$$
$$2(C_{A1} - C_{A2}) - r_{A2}V_2 = 0$$
$$2(C_{A2} - C_{A3}) - r_{A3}V_3 = 0$$
$$r_{A1} - C_{A1}^{1.5} = 0$$
$$r_{A2} - C_{A2}^{1.5} = 0$$
$$r_{A3} - C_{A3}^{1.5} = 0$$

Model equation

$$V_1 + V_2 + V_3 \le 7$$

Linear inequality constraint

$$V = [V_1, V_2, V_3]^T$$

Reactors in Series: MATLAB Program

Write the model equation of the system in a function file

$$r_{A1} = C_{A1}^{1.5}$$
$$r_{A2} = C_{A2}^{1.5}$$
$$r_{A3} = C_{A3}^{1.5}$$

$$2(C_{A0} - C_{A1}) - r_{A1}V_1 = 0$$
$$2(C_{A1} - C_{A2}) - r_{A2}V_2 = 0$$
$$2(C_{A2} - C_{A3}) - r_{A3}V_3 = 0$$

```
function F = CSTR(CA)
global V

F0 = 2;      % Flow rate
k = 1;       % Reaction constant
CA0 = 1;     % Initial concentration of reactant A
V1 = V(1);   % Volume of reactor 1
V2 = V(2);   % Volume of reactor 2
V3 = V(3);   % Volume of reactor 3

% Reaction rates
R1 = k*CA(1)^1.5;
R2 = k*CA(2)^1.5;
R3 = k*CA(3)^1.5;

% Model equations
F(1) = F0*(CA0 - CA(1))-V1*R1;
F(2) = F0*(CA(1) - CA(2))-V2*R2;
F(3) = F0*(CA(2) - CA(3))-V3*R3;
end
```

Reactors in Series: MATLAB Program

Objective: Find CSTR volumes to minimize C_{A3}. We have to solve CSTR models to find C_{A3}.

Solve the model equations and define the objective function in another function file

```
function f = objfun(Vol)
global V

V = Vol;  % Volume of all three reactors

CA_guess = [1 1 1]; % Initial guess value of concentration

CA = fsolve(@CSTR,CA_guess); % Solve model equations

f = CA(3); % Objective function
end
```

Reactors in Series

Now write this code in MATLAB command window (or write a script)

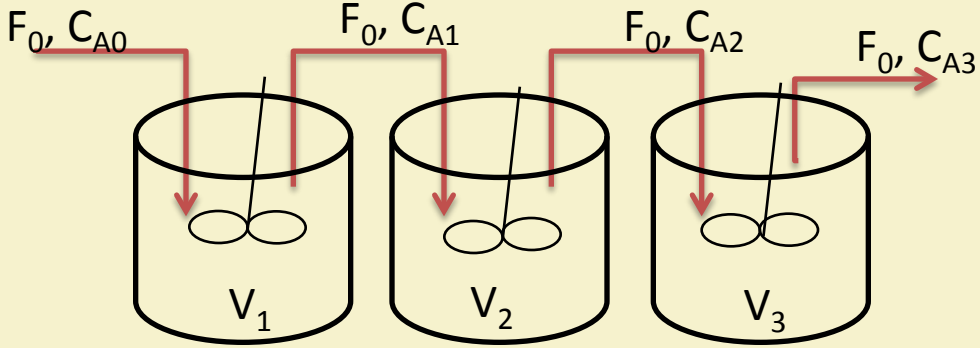
Solve the optimization problem using MATLAB function `fmincon`

```
V0 = [2 3 2]; % Initial guess value of volume [V1 V2 V3]

A = [1 1 1];  % Linear inequality constraint
b = 7;

Aeq = [];
beq = [];
lb = [];
ub = [];
Options = optimset('Algorithm','interior-
point','MaxIter',1000,'MaxFunEvals',10000,'Display','iter');
[V, fval] = fmincon(@objfun,V0,A,b,Aeq,beq,lb,ub,[],options);

% display results
fprintf('V1 = %f \n', V(1))
fprintf('V2 = %f \n', V(2))
fprintf('V2 = %f \n', V(3))
fprintf('The optimal value of CA3 = %f \n', fval)
```

Reactors in Series

Result

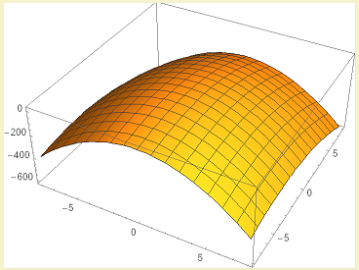
```
V1 = 2.077897
V2 = 2.331545
V2 = 2.590543
The optimal value of CA3 = 0.210472
```



$V_1 = 2.0779\ m^3$ $V_2 = 2.3315\ m^3$ $V_3 = 2.5905\ m^3$

$C_{A3} = 0.2105$ **kmol/m³**

Optimization in Chemical Engineering



Thank You

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OPTIMIZATION IN CHEMICAL ENGINEERING

Applications of Optimization

(WEEK – 11: LECTURE – 52)

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Applications of Optimization

Week 11:

- Optimization of various chemical and biochemical processes

Example-1

Continuous Stirred Tank Reactors (CSTR) in Series:

What should be the number of reactors so that the cost is minimized?

Optimum Number of Reactors: The Problem

Consider first order reaction

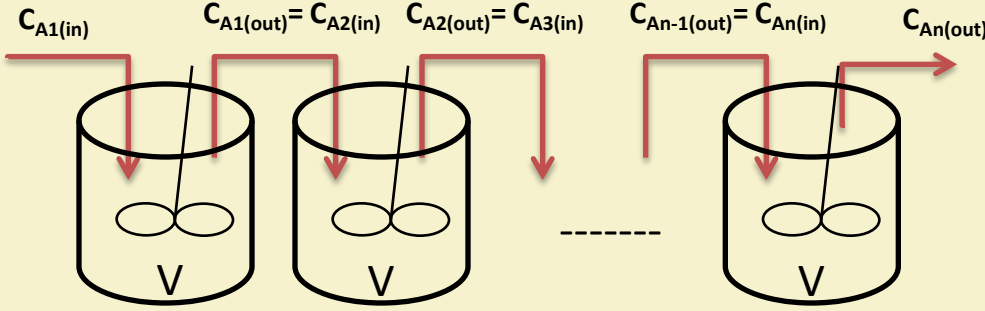
A → Product

The design equation for the CSTR is

$$C_{Ai(\text{out})} = \frac{C_{Ai(\text{in})}}{1 + \frac{kV}{Q}}, \quad i \in 1, 2, 3, \ldots\ldots n$$

The cost of a reactor depends on its volume (V m^3) and is expressed as:

$$\text{Cost} = 137000\left(V^{0.4}\right)$$



Volumetric flow rate of liquid, Q = 0.9 m^3/hr

First order rate constant , k = 12 hr^{-1}

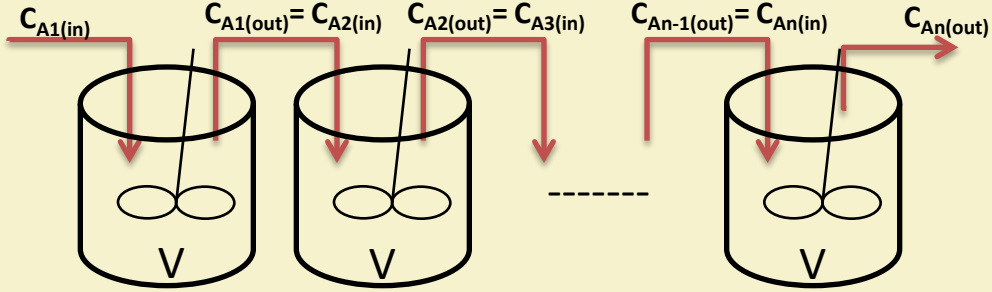
Desired concentration change:

$$\frac{C_{A1(\text{in})}}{C_{An(\text{out})}} = 10000$$

Determine the optimum number of reactors so that the cost is minimum.

Optimum Number of Reactors: Formulation

$$C_{Ai(out)} = \frac{C_{Ai(in)}}{1+\frac{kV}{Q}}, \quad i \in 1,2,3,.....n$$



Note:

$$C_{A1(out)} = C_{A2(in)}, \ldots\ldots, C_{A(n-1)(out)} = C_{An(in)}$$

$$C_{Ai(out)} = \frac{C_{Ai(in)}}{1+\frac{kV}{Q}} = \left(1+\frac{kV}{Q}\right)^{-1} C_{A(i-1)(out)}, \quad i \in \{2,3,.....n\}$$

Applying recursively,

$$C_{An(out)} = \left(1+\frac{kV}{Q}\right)^{-n} C_{A1(in)}$$

$$\frac{C_{A1(in)}}{C_{An(out)}} = 10000$$

$$\Rightarrow \left(1+\frac{kV}{Q}\right)^{n} = 10000$$

$$\Rightarrow V = \frac{Q}{k}\left(\sqrt[n]{10000}-1\right) = \frac{40}{3}\left(\sqrt[n]{10000}-1\right)$$

$Q = 0.9\ m^3/hr$

$k = 12\ hr^{-1}$

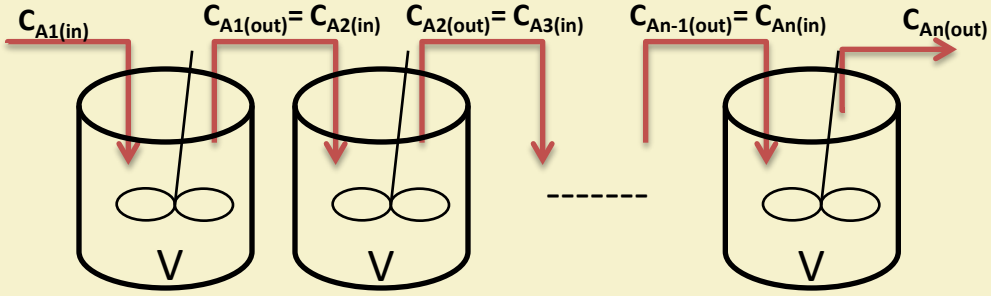
Optimum Number of Reactors: Formulation

$$\text{Reactor cost} = 137000\left(V^{0.4}\right)$$

The cost function for *n* reactors is expressed by

$$\text{Cost} = (n)137000\left(V^{0.4}\right)$$

$$= (137000n)\left[\frac{40}{3}\left(\sqrt[n]{10000} - 1\right)\right]^{0.4}$$



Objective function:

$$\underset{n}{\text{minimize}} \quad \text{Cost} = (137000n)\left[\frac{40}{3}\left(\sqrt[n]{10000} - 1\right)\right]^{0.4}$$

Optimum Number of Reactors: MATLAB Program

Write the equation for cost function in a function file as follows:

```
function C = Cost(n)
C = 137000*n*((40/3)*((10000)^(1/n)-1))^(2/5); % Cost function
end
```

Now enter the following on MATLAB command window (or write a script):

```
n0 = 2; % Initial guess
options = optimset('Display','iter','TolFun',1e-8);
[n, fval] = fminsearch(@Cost,n0,options);
fprintf('n = %f \n', n)
fprintf('The optimal cost = %f \n', fval)
```

Result:

```
n = 4.127214
The optimal cost = 3717878.815866
```

Optimum number of reactors = 4

$$V = \frac{Q}{k}\left(\sqrt[n]{10000} - 1\right)$$

$$= \frac{40}{3}\left(\sqrt[4]{10000} - 1\right) = 120 \text{ m}^3$$

Example-2

Optimal Diameter of a Pipe

Optimal Pipe Diameter

In a chemical plant, the cost of pipes, their fittings, and pumping are important investment. Consider the design of a pipeline L ft long that should carry fluid at the rate of Q gpm. The selection of economic pipe diameter D (inch) is based on minimizing the annual cost of pipe, pump, and pumping. Suppose the annual cost of a pipeline with a standard carbon steel pipe and a motor-driven centrifugal pump can be expressed as:

$$Cost = 0.45L + 0.245LD^{1.5} + 3.25(hp)^{1/2} + 61.6(hp)^{0.925} + 102$$

where $$hp = 4.4\times10^{-8}\frac{LQ^3}{D^5} + 1.92\times10^{-9}\frac{LQ^{2.68}}{D^{4.68}}$$

Formulate the appropriate single-variable optimization problem for designing a pipe of length 1000 ft with a fluid rate of 20 gpm so that the cost is minimum. The diameter of the pipe should be between 0.25 to 6 inch.

Optimal Pipe Diameter: Problem Formulation

Objective function:

$$\underset{D}{\text{minimize}} \quad Cost = 0.45(1000) + 0.245(1000)D^{1.5} + 3.25\left[4.4\times10^{-8}\frac{(1000)(20)^3}{D^5} + 1.92\times10^{-9}\frac{(1000)(20)^{2.68}}{D^{4.68}}\right]^{1/2}$$

$$+61.6\left[4.4\times10^{-8}\frac{(1000)(20)^3}{D^5} + 1.92\times10^{-9}\frac{(1000)(20)^{2.68}}{D^{4.68}}\right]^{0.925} + 102$$

Subject to $2.5 < D < 6$

Optimal Pipe Diameter: MATLAB Program

Write the equation for cost in a function file as follows:

```
function f = Pipedia(D)

L = 1000; % length of pipe (ft)
Q = 20; % flow rate (gpm)

hp=4.4e-8*(L*Q^3)/D^5 + 1.92e-9*(L*Q^2.68) /(D^4.68);

f=0.45*L+0.245*L*D^1.5+3.25*hp^0.5+61.6*hp^0.925+102;
end
```

Optimal Pipe Diameter: MATLAB Program

Now write this on MATLAB command window (or write a script):

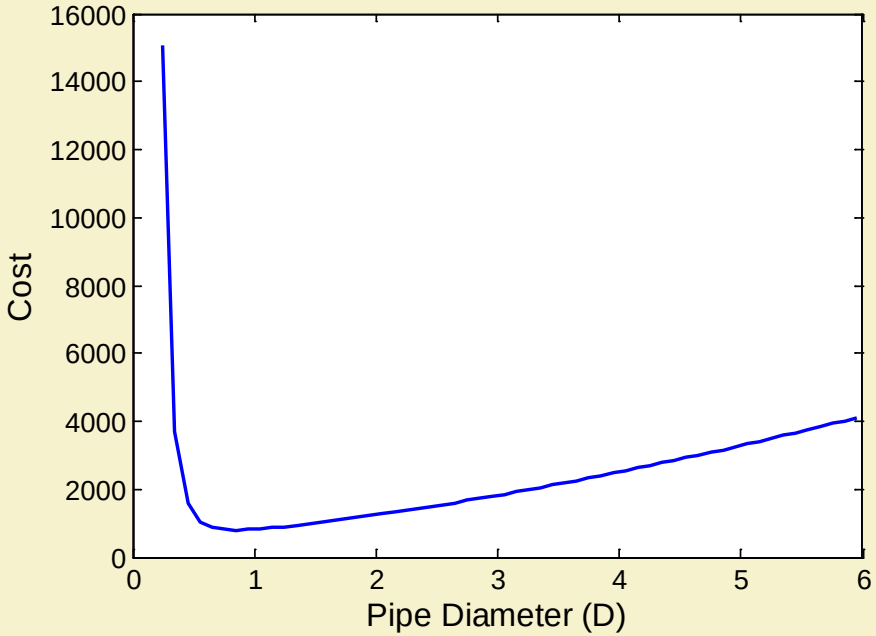
```
D0 = 0.3; % initial guess value
A = [];
b1 = [];
Aeq = [];
beq = [];
lb =0.25;
ub = 6;
options=optimset('Algorithm','interior-
point','MaxIter',1000,'MaxFunEvals',10000,'Display','iter');
[D, fval] = fmincon(@Pipedia,D0,A,b1,Aeq,beq,lb,ub,[],options);
fprintf('D = %f \n', D)
fprintf('The optimal cost = %f \n', fval)
```

Result:

```
D = 0.825033
The optimal cost
= 796.649325
```

Diameter = 0.8250 in.

Optimal Pipe Diameter: Optimization Results

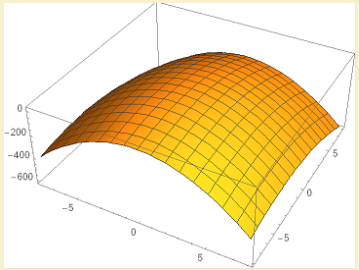


Result:

```
D = 0.825033
The optimal cost
= 796.649325
```

Diameter = 0.8250 in.

Optimization in Chemical Engineering



Thank You

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Week 11:

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MATLAB Function `fminbnd`

The MATLAB function `fminbnd` finds minimum of single-variable function on fixed interval.

$$\underset{x}{\text{Minimize}} \quad f(x)$$

$$\text{Such that:} \quad x_1 < x < x_2$$

Here, x, x_1, and x_2 are finite scalars, and $f(x)$ is a function that returns a scalar.

MATLAB Function fminbnd : Syntax

```
x = fminbnd(fun,x1,x2)
x = fminbnd(fun,x1,x2,options)
```

```
[x,fval] = fminbnd(___)
[x,fval,exitflag] = fminbnd(___)
[x,fval,exitflag,output] = fminbnd(___)
```

"fval" returns the value of the objective function computed in "fun" at the solution x.

"exitflag" describes the exit condition.

"output" returns a structure output that contains information about the optimization.

More information at:

https://in.mathworks.com/help/optim/ug/fminbnd.html

MATLAB Function `fminbnd` : Algorithm

The algorithm is based on golden section search and parabolic interpolation.

Note:

- The function to be minimized must be continuous.
- `fminbnd` may converge to local solutions.
- `fminbnd` can exhibit slow convergence when the solution is on a boundary of the interval. In such a case, `fmincon` often gives faster and more accurate solutions.

More information at:

https://in.mathworks.com/help/optim/ug/fminbnd.html

MATLAB Function fminbnd : Example

$$\underset{x}{\text{Minimize}} \quad f(x) = x^2 - 2$$

$$\text{Such that:} \quad -2 < x < 2$$

First write a function file to evaluate objective function:

```
function f = myfun(x)
f = x*x - 2;          % Compute function value at x.
end
```

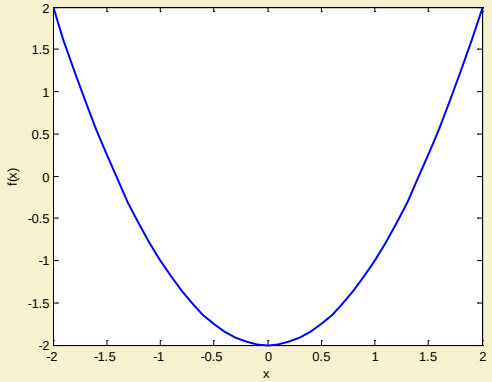
Now call the optimization solver:

```
options = optimset('Display','iter'); % Option to display output
[x, fval] = fminbnd(@myfun,-2,2,options)
```

MATLAB Function fminbnd : Example

$$\underset{x}{\text{Minimize}} \quad f(x) = x^2 - 2$$

$$\text{Such that:} \quad -2 < x < 2$$




```
Func-count     x          f(x)          Procedure
    1      -0.472136     -1.77709         initial
    2       0.472136     -1.77709         golden
    3         1.05573    -0.885438         golden
    4   -5.55112e-17            -2         parabolic
    5    3.33333e-05            -2         parabolic
    6   -3.33333e-05            -2         parabolic

Optimization terminated:
the current x satisfies the termination criteria using
OPTIONS.TolX of 1.000000e-04

x = -5.5511e-17

fval = -2
```

MATLAB Function `fminbnd` : Alternate Use

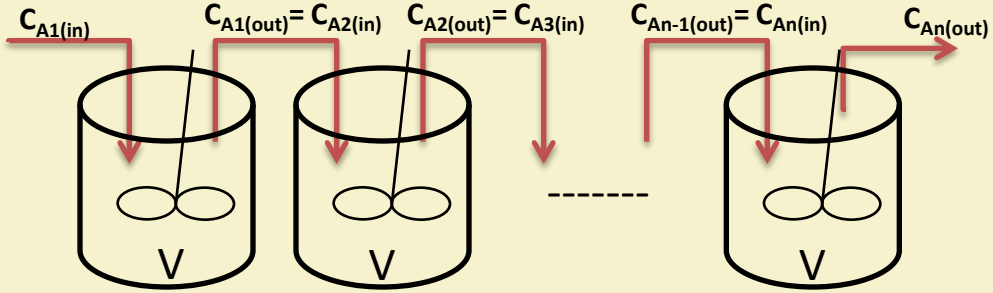
$$\underset{x}{\text{Minimize}} \quad f(x) = x^2 - 2$$

$$\text{Such that:} \quad -2 < x < 2$$

The argument `fun` can also be a function handle for an anonymous function.

```
f = @(x)x.^2 - 2;

options = optimset('Display','iter'); % Option to display output
[x, fval] = fminbnd(f,-2,2,options)
```

Optimum Number of Reactors: Revisit Lecture 51



Find the optimum number of CSTR that minimizes the total cost.

Objective function:

$$\underset{n}{\text{minimize}} \quad \text{Cost} = (137000n)\left[\frac{40}{3}\left(\sqrt[n]{10000}-1\right)\right]^{0.4}$$

Optimum Number of Reactors: fminbnd

Write the equation for cost function in a function file as follows:

```
function C = Cost(n)
C = 137000*n*((40/3)*((10000)^(1/n)-1))^(2/5); % Cost function
end
```

Now enter the following on MATLAB command window (or write a script):

```
x1 = 1; x2 = 10; % The bounds on
options = optimset('Display','iter','TolFun',1e-8);
[n, fval] = fminbnd(@Cost,x1,x2,options);
fprintf('n = %f \n', n)
fprintf('The optimal cost = %f \n', fval)
```

Result:

```
n = 4.127203
The optimal cost = 3717878.815876
```

Optimum number of reactors = 4

$$V = \frac{Q}{k}\left(\sqrt[n]{10000} - 1\right)$$

$$= \frac{40}{3}\left(\sqrt[4]{10000} - 1\right) = 120 \text{ m}^3$$

MATLAB Function fminbnd : Example

Func-count	x	f(x)	Procedure
1	4.43769	3.72482e+06	initial
2	6.56231	3.96808e+06	golden
3	3.12461	3.83879e+06	golden
4	4.52231	3.72883e+06	parabolic
5	4.23333	3.71875e+06	parabolic
6	3.80984	3.7269e+06	golden
7	4.14498	3.7179e+06	parabolic
8	4.12012	3.71788e+06	parabolic
9	4.12704	3.71788e+06	parabolic
10	4.12724	3.71788e+06	parabolic
11	4.1272	3.71788e+06	parabolic
12	4.12717	3.71788e+06	parabolic

```
Optimization terminated:
the current x satisfies the termination criteria
using OPTIONS.TolX of 1.000000e-04

n = 4.127203     The optimal cost = 3717878.815876
```

Compare the solution obtained with `fminsearch`

```
n = 4.127214

The optimal cost =
3717878.815866
```

Optimal Pipe Diameter: Revisit Lecture 53

Objective function:

$$\underset{D}{\text{minimize}} \quad Cost = 0.45(1000) + 0.245(1000)D^{1.5} + 3.25\left[4.4\times10^{-8}\frac{(1000)(20)^3}{D^5} + 1.92\times10^{-9}\frac{(1000)(20)^{2.68}}{D^{4.68}}\right]^{1/2}$$

$$+61.6\left[4.4\times10^{-8}\frac{(1000)(20)^3}{D^5} + 1.92\times10^{-9}\frac{(1000)(20)^{2.68}}{D^{4.68}}\right]^{0.925} + 102$$

Subject to $2.5 < D < 6$

Optimal Pipe Diameter: Solve Using fminbnd

Write the equation for cost in a function file as follows:

```
function f = Pipedia(D)

L = 1000; % length of pipe (ft)
Q = 20; % flow rate (gpm)

hp=4.4e-8*(L*Q^3)/D^5 + 1.92e-9*(L*Q^2.68) /(D^4.68);

f=0.45*L+0.245*L*D^1.5+3.25*hp^0.5+61.6*hp^0.925+102;
end
```

Optimal Pipe Diameter: Solve Using `fminbnd`

Now write this on MATLAB command window (or write a script):

```
D1 = 0.25; D2 = 6.0; % The bounds on pipe diameter
Options = optimset('Display','iter');
[D, fval] = fminbnd(@Pipedia, D1, D2, options);
fprintf('D = %f \n', D)
fprintf('The optimal cost = %f \n', fval)
```

Result:

```
D = 0.825048
The optimal cost
= 796.649326
```

Diameter = 0.8250 in.

MATLAB Function fminbnd : Example

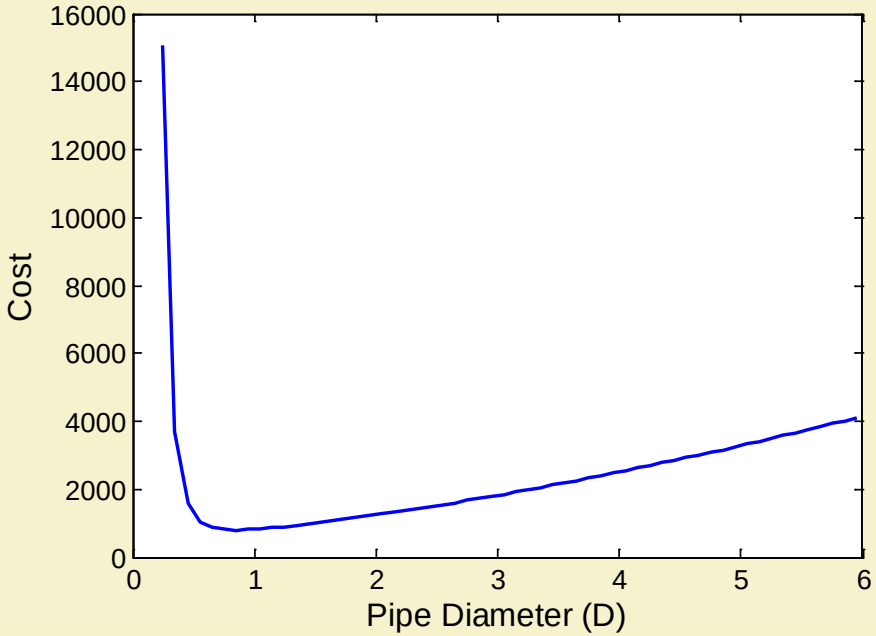
Func-count	x	f(x)	Procedure
1	2.4463	1490.01	initial
2	3.8037	2369.62	golden
3	1.60739	1054.54	golden
4	1.08891	848.029	golden
5	0.768477	801.195	golden
6	0.685558	832.312	parabolic
7	0.872166	799.088	parabolic
8	0.954956	812.279	golden
9	0.830868	796.69	parabolic
10	0.828408	796.663	parabolic
11	0.824468	796.65	parabolic
12	0.825015	796.649	parabolic
13	0.825048	796.649	parabolic
14	0.825082	796.649	parabolic

```
Optimization terminated:
the current x satisfies the termination criteria using OPTIONS.TolX of 1.000000e-04

D = 0.825048
The optimal cost = 796.649326
```

Compare the solution obtained with `fmincon`

```
D = 0.825033

The optimal cost =
796.649325
```

Optimal Pipe Diameter: Optimization Results

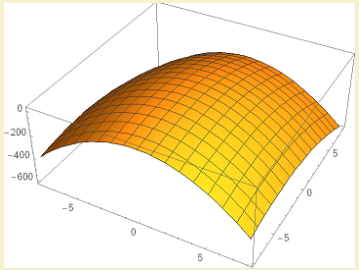


Result:

```
D = 0.825048
The optimal cost
= 796.649326
```

Diameter = 0.8250 in.

Optimization in Chemical Engineering



Thank You

IIT KHARAGPUR

NPTEL ONLINE CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Applications of Optimization

(WEEK – 11: LECTURE – 54)

Dr. Debasis Sarkar

Department of Chemical Engineering

Indian Institute of Technology Kharagpur

Applications of Optimization

Week 11:

- Optimization of various chemical and biochemical processes

Example-1

Optimization of a Continuous Stirred Tank Reactor (CSTR)

For a given product specification, what should be the volume, feed-rate, and reactor concentration so that the total operating cost is minimized?

Optimization of a CSTR: Problem Statement

A feed stream carrying only reactant *A* with concentration C_{A0} mol/m^3 enters a CSTR with volumetric feed-rate *F* m^3/h and undergoes a first order reaction *A* → *B*.

The rate of formation of B is given as $r_B = kC_A$

where $k = 0.1$ h^{-1} is the reaction rate constant.

We wish to produce 10 mol/h of *B* and cost of this operation per hour (C_T Rs/h) can be expressed as sum of two cost components: cost of feed *A* and cost of utility that depends on CSTR volume (V m^3), as follows:

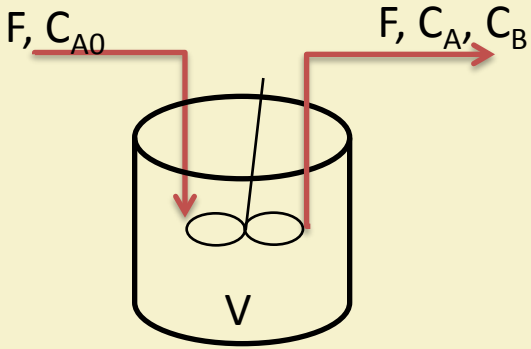
$$C_T = 5C_{A0}F + 0.3V$$

If the initial concentration of A, $C_{A0} = 0.04$ mol/m^3, find the minimum cost of operation.

Optimization of a CSTR: How to Solve?

In order to minimize the cost of operation, we need to determine the optimal values of reactor volume (V), feed rate (F), and concentration of A in the reactor (C_A). Formulate a constrained optimization problem to determine optimal V, F and C_A. Use mass balance equations on A and B to formulate these constraints. Use method of Lagrange multipliers to derive the expressions for optimal V, F, and C_A.

Material Balance: Accumulation = Input - Output



Optimization of a CSTR: Formulation

Material Balance: Accumulation = Input - Output

Material balance on A

$$0 = C_{A0}F - \left(r_A V + FC_A\right)$$

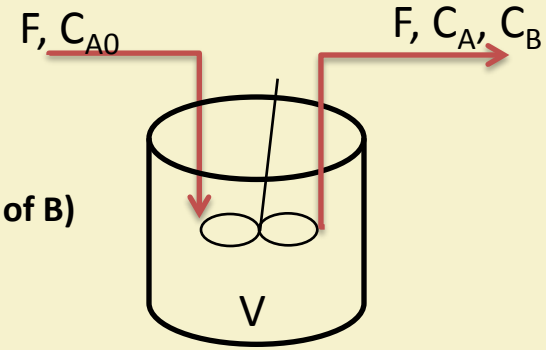
$$\Rightarrow \left(C_{A0} - C_A\right)F - 0.1C_A V = 0$$

Material balance on B

$$0 = r_B V - FC_B$$

$$\Rightarrow 0.1C_A V - 10 = 0$$

(Because we want to produce 10 mol/h of B)



Note: $r_B = kC_A$ where k = 0.1 h^{-1}

Optimization Problem Formulation:

Minimize $C_T = 5C_{A0}F + 0.3V$

Subject to $\left(C_{A0} - C_A\right)F - 0.1C_A V = 0$

$$0.1C_A V - 10 = 0$$

Optimization of a CSTR

The Lagrangian Function

$$L = \left[5C_{A0}F + 0.3V\right] + \lambda_1\left[\left(C_{A0} - C_A\right)F - 0.1C_AV\right] + \lambda_2\left[0.1C_AV - 10\right]$$

$$\frac{\partial L}{\partial F} = 5C_{A0} + \lambda_1\left(C_{A0} - C_A\right) = 0$$

$$\frac{\partial L}{\partial V} = 0.3 - 0.1\lambda_1C_A + 0.1\lambda_2C_A = 0$$

$$\frac{\partial L}{\partial C_A} = -\lambda_1F - 0.1\lambda_1V + 0.1\lambda_2V = 0$$

$$\frac{\partial L}{\partial \lambda_1} = \left(C_{A0} - C_A\right)F - 0.1C_AV = 0$$

$$\frac{\partial L}{\partial \lambda_2} = 0.1C_AV - 10 = 0$$

Optimization of a CSTR

The Lagrangian Function $L = [5C_{A0}F + 0.3V] + \lambda_1[(C_{A0} - C_A)F - 0.1C_AV] + \lambda_2[0.1C_AV - 10]$

$$\frac{\partial L}{\partial F} = 5C_{A0} + \lambda_1(C_{A0} - C_A) = 0$$

$$\frac{\partial L}{\partial V} = 0.3 - 0.1\lambda_1 C_A + 0.1\lambda_2 C_A = 0$$

$$\frac{\partial L}{\partial C_A} = -\lambda_1 F - 0.1\lambda_1 V + 0.1\lambda_2 V = 0$$

$$\frac{\partial L}{\partial \lambda_1} = (C_{A0} - C_A)F - 0.1C_AV = 0$$

$$\frac{\partial L}{\partial \lambda_2} = 0.1C_AV - 10 = 0$$

Solve these equations simultaneously using MATLAB function `fsolve`

$f(x) = 0$

```
[x, fval] = fsolve(fun,x0,options)
```

Optimization of a CSTR: Solution

```
function L = CSTR_Lagrangian(X)
CA0 = 0.04;
F = X(1);
V = X(2);
CA = X(3);
lambda1 = X(4);
lambda2 = X(5);
% Equation
L(1) = 5*CA0 + lambda1*(CA0-CA);
L(2) = 0.3 - lambda1*0.1*CA +
lambda2*0.1*CA;
L(3) = -lambda1*F-
lambda1*0.1*V+lambda2*0.1*V;
L(4) = (CA0-CA)*F - 0.1*CA*V;
L(5) = 0.1*CA*V - 10;
end
```

```
X_guess = [1000 1000 0.04 0 0]; % initial
guess value
options =
optimoptions('fsolve','Display','iter','MaxFun
Evals',1000000,'MaxIter',100000,'TolFun',1e-
8);
X = fsolve(@CSTR_Lagrangian,X_guess,options);
% Solve equations
```

F	12182 m^3/h
V	31455 m^3
C_A	0.0318 mol/m^3

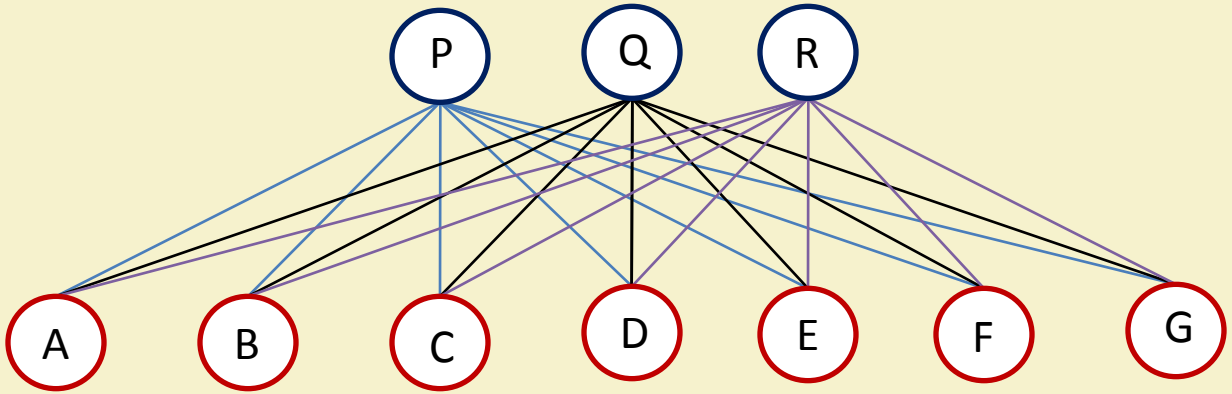
$$C_T = 5C_{A0}F + 0.3V$$
$$= 11872.9 \text{ Rs/h}$$

Example-2

Optimization of Transportation Cost

Transportation Cost Optimization

A manufacturing company delivers a product from its three warehouses in P, Q and R to seven distributor's warehouses in A, B, C, D, E, F, and G.



`linprog` solves:

$$\underset{x}{\text{Minimize}} \quad f^T x$$

$$\text{Such that: } A \cdot x \leq b$$

$$A_{eq} = b_{eq}$$

$$LB \leq x \leq UB$$

Transportation Cost Optimization: Data

The shipping costs of a product from company's warehouse to different distributor's warehouses are given in the table below:

Distributor warehouse \ Company warehouse	P	Q	R
A	15	160	100
B	160	12	260
C	154	315	56
D	245	410	190
E	130	290	58
F	125	427	204
G	215	375	160

Demand at different distributor's warehouses:

A	1168
B	1560
C	1439
D	986
E	1658
F	2035
G	1159

Storage capacity of company's different warehouses:

P	3980
Q	1785
R	4856

Solve the linear programming problem to find the optimal quantity of product to be delivered to each distributor's warehouse so that the total transportation cost will be minimum.

Transportation Cost Optimization: Formulation

Shipping Costs

	A	B	C	D	E	F	G
P	C1 = 15	C2 = 160	C3 = 154	C4 = 245	C5 = 130	C6 = 125	C7 = 215
Q	C8 = 160	C9 = 12	C10 = 315	C11 = 410	C12 = 290	C13 = 427	C14 = 375
R	C15 = 100	C16 = 260	C17 = 56	C18 = 190	C19 = 58	C20 = 204	C21 = 160

Shipments

	A	B	C	D	E	F	G	Total Out		Stock
P	x1	x2	x3	x4	x5	x6	x7	x1+x2+x3+x4+x5+x6+x7	≤	3980
Q	x8	x9	x10	x11	x12	x13	x14	x8+x9+x10+x11+x12+x13+x14	≤	1785
R	x15	x16	x17	x18	x19	x20	x21	x15+x16+x17+x18+x19+x20+x2	≤	4856
Total In	x1+x8+x15	x2+x9+x16	x3+x10+x17	x4+x11+x18	x5+x12+x19	x6+x13+x20	x7+x14+x21			
	II	II	II	II	II	II	II			
Requirement	1168	1560	1439	986	1658	2035	1159			

Objective function $\underset{x}{\text{Minimize}} \quad \text{Cost} = \sum_{i=1}^{21} C_i x_i$

Transportation Cost Optimization: MATLAB Code

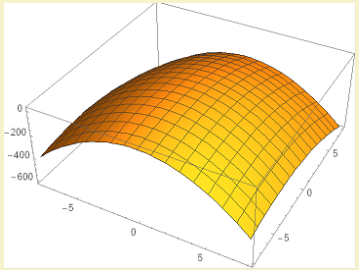
```
f = [15 160 154 245 130 125 215 160 12  315 410 290 427 375 100 260 56
190 58  204 160];
A = [1 1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
     0 0 0 0 0 0 0 1 1 1 1 1 1 1 0 0 0 0 0 0 0;
     0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1];
b = [3980; 1785; 4856];
lb = [0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0];
ub = 5000.*ones(1,21);
Aeq = [1 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0;
       0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0;
       0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0;
       0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0;
       0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0;
       0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0;
       0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 1];
beq = [1168; 1560; 1439; 986; 1658; 2035; 1159];
[x, fval] = linprog(f,A,b,Aeq,beq,lb,ub)
```

Transportation Cost Optimization: Solution

			Shipments							
	A	B	C	D	E	F	G	Total Out		Stock
P	1168	0	0	386	0	2035	0	3589	≤	3980
Q	0	1560	0	0	0	0	0	1560	≤	1785
R	0	0	1439	600	1658	0	1159	4856	≤	4856
Total In	1168	1560	1439	986	1658	2035	1159			
	II	II	II	II	II	II	II			
Requirement	1168	1560	1439	986	1658	2035	1159			

The optimal cost = $\sum_{i=1}^{21} C_i x_i = 861373$

Optimization in Chemical Engineering



Thank You

IIT KHARAGPUR

NPTEL ONLINE CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Applications of Optimization

(WEEK – 11: LECTURE – 55)

Dr. Debasis Sarkar

Department of Chemical Engineering

Indian Institute of Technology Kharagpur

Applications of Optimization

Week 11:

- Optimization of various chemical and biochemical processes

Example

Optimization of a Continuous Bioreactor: Microbial Growth in a Chemostat

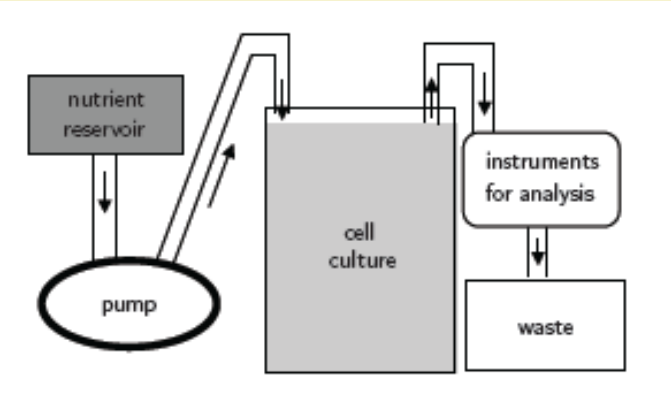
Optimization of a Continuous Bioreactor

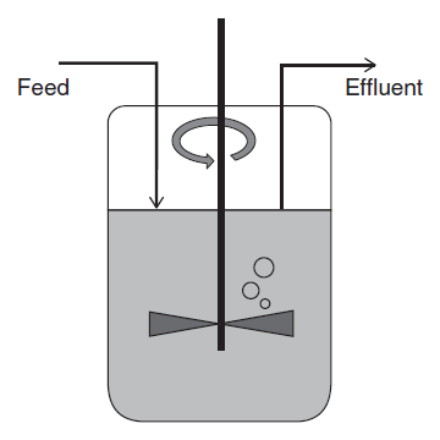
A chemostat is a continuous stirred-tank bioreactor.

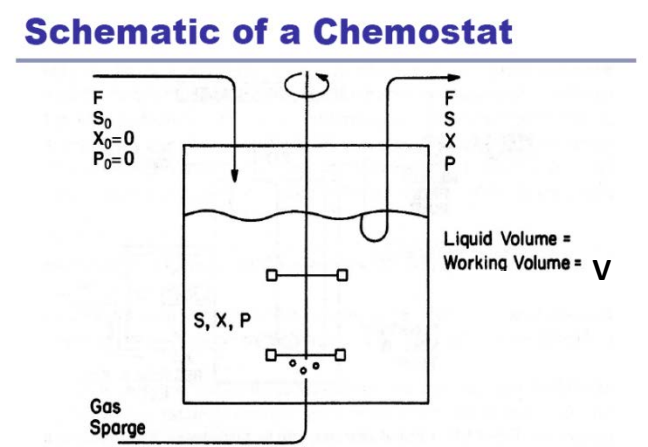
It consists of a fresh water and nutrient reservoir connected to a growth chamber (bioreactor), with microorganisms. The mixture of fresh water and nutrient is pumped continuously from the reservoir to the reactor, providing feed to the microorganisms. The mixture of culture and fluid in the bioreactor is continuously pumped out and collected.

The medium culture is continuously stirred. Stirring ensures that the contents of the bioreactor is well mixed so that the culture production is uniform and steady. If the strring speed is too high, it would damage the cells in culture, but if it is too low it could prevent the reactor from reaching a steady state operation.

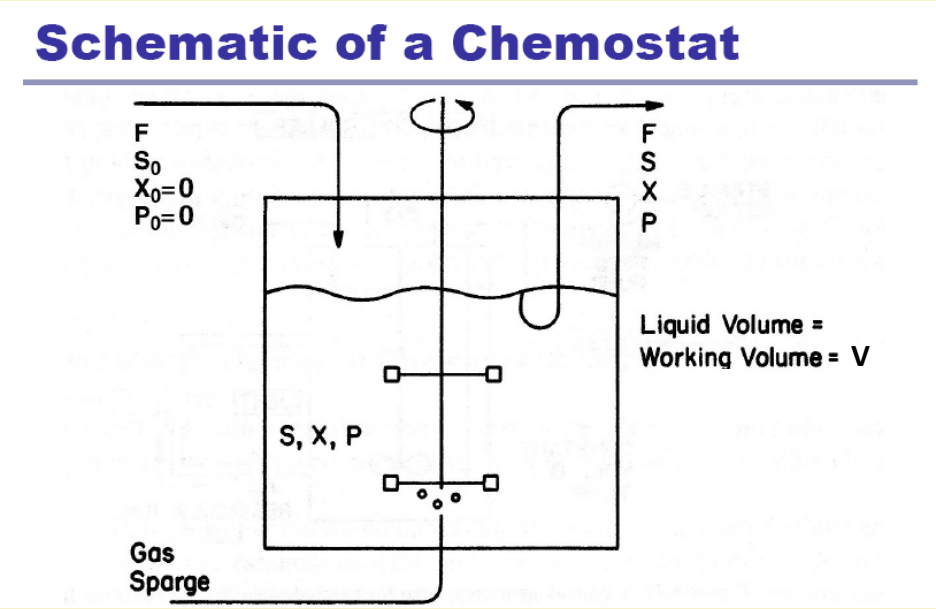
Continuous Bioreactor: Schematic Representation







Applications of Continuous Bioreactors

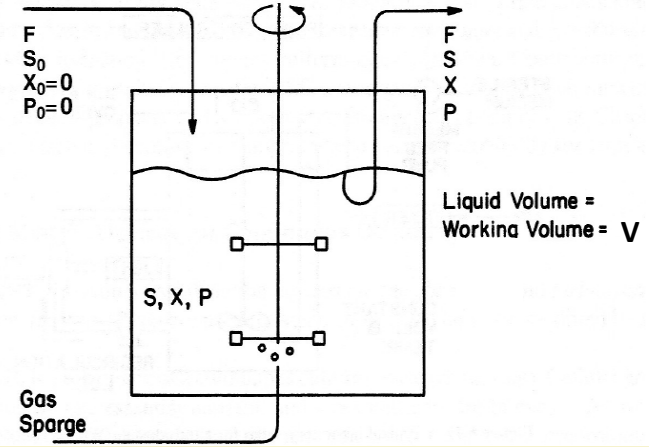


The stirred-tank bioreactor is one of the most commonly used types for large scale production in industrial applications such as food, pharmaceuticals, various commodity and specialty chemicals.

The chemostat is a widely-used apparatus for the study of microbial physiology.

Features of a Chemostat

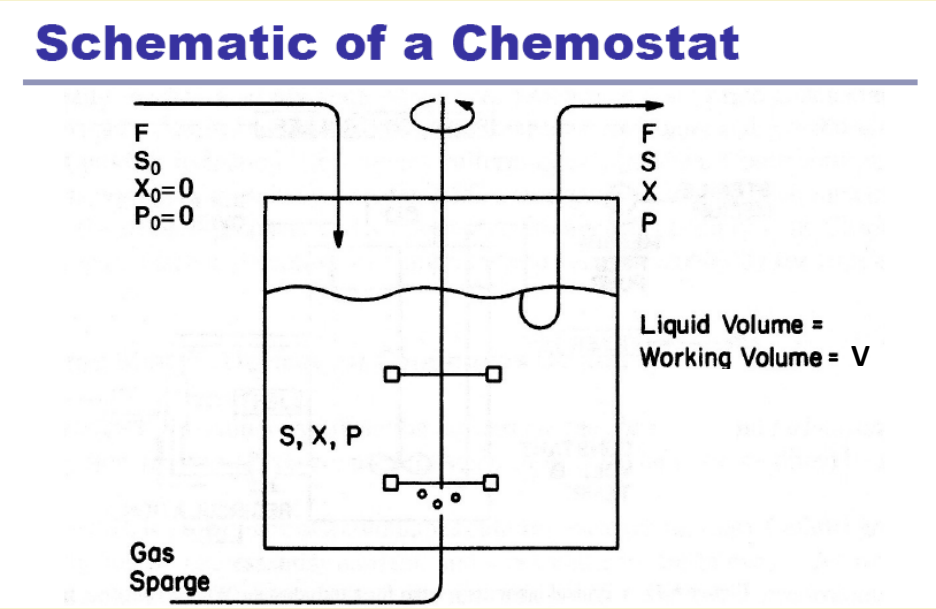
Schematic of a Chemostat



A chemostat is a continuous bioreactor where

- a fresh medium is continuously introduced at a constant rate,
- the culture volume is kept constant by continuous removal of culture at the same rate,
- the supply of a single nutrient controls growth rate.

Continuous Bioreactor: Nomenclature

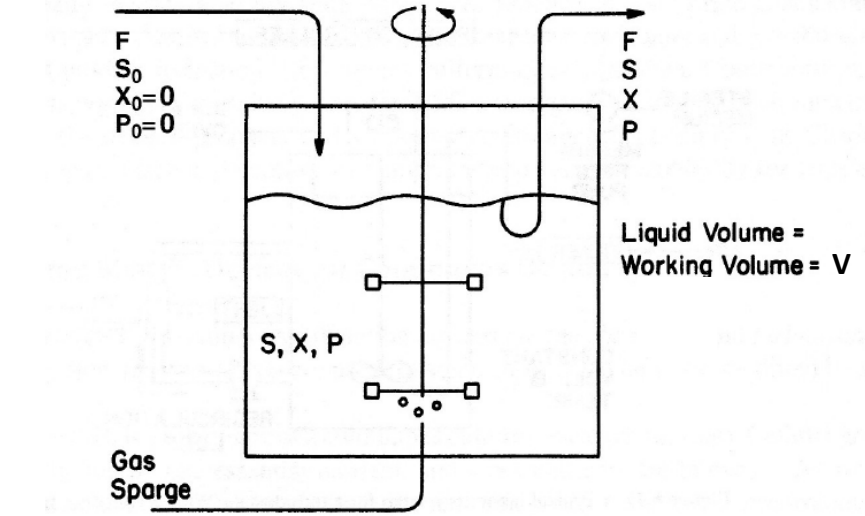


F = Volumetric flow rate
V = Volume of bioreactor
X = Biomass concentration, biomass/volume
S = Substrate concentration, mass/volume
P = Product concentration, mass/volume
S_0 = Feed substrate concentration, mass/volume
X_0 = Biomass concentration in feed stream
= zero for sterile feed
P_0 = Product concentration in the feed stream

$F_{in} = F_{out} = F \neq 0$
V = constant

Optimization of a Continuous Bioreactor

Schematic of a Chemostat



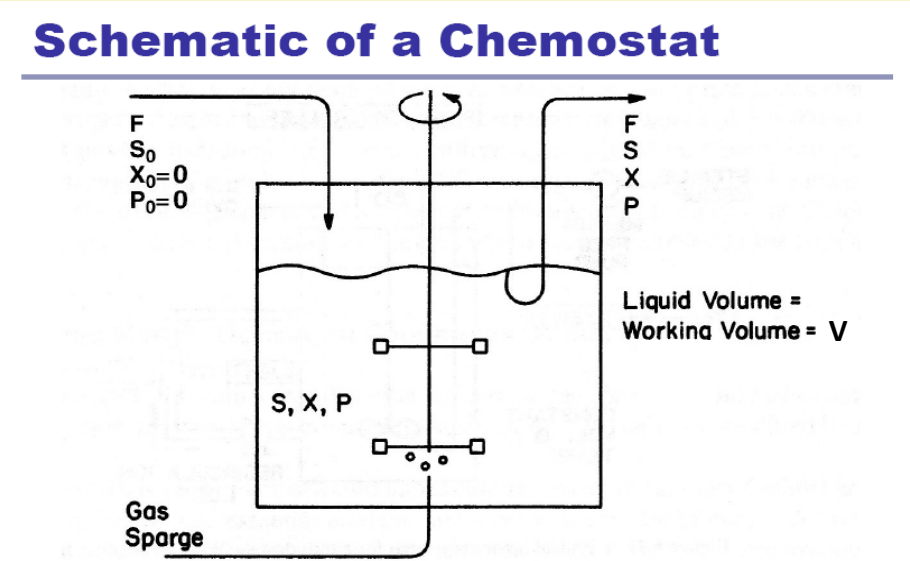
One can manipulate:

1. Concentration of a limiting nutrient
2. Dilution rate, D = F/V

Both influences X and P

Dilution rate determines the specific growth rate of the culture.

Optimization of a Continuous Bioreactor: Modeling



$$\frac{d(XV)}{dt} = \mu(XV) - F(XV)$$

$$\frac{d(SV)}{dt} = FS_0 - FS - \sigma(XV) = F(S_0 - S) - \sigma(XV)$$

From above:

$$\frac{dX}{dt} = \mu X - DX$$

$$\frac{dS}{dt} = \frac{F}{V}(S_0 - S) - \sigma X$$

$$\Rightarrow \frac{dS}{dt} = D(S_0 - S) - \sigma X$$

Monod kinetics:

$$\mu = \frac{\mu_{max} S}{K_s + S}$$

$$D = \frac{F}{V}$$

$$\sigma = \frac{\mu}{Y_{x/s}}$$

Optimization of a Continuous Bioreactor

$$\frac{dX}{dt} = \mu X - DX$$

$$\frac{dS}{dt} = D(S_0 - S) - \sigma X$$

At steady state: $\mu X = DX$

$$\Rightarrow \mu = D$$

$$\Rightarrow D = \frac{\mu_{max} S}{K_s + S}$$

$$D(S_0 - S) - \sigma X = 0$$

Monod kinetics:

$$\mu = \frac{\mu_{max} S}{K_s + S}$$

$$D = \frac{F}{V}$$

$$\sigma = \frac{\mu}{Y_{x/s}}$$

Thus, by varying the dilution rate (or the feed flow rate), the growth rate can be controlled.

We can write:

$$S = \frac{K_s \mu}{\mu_{max} - \mu} = \frac{DK_s}{\mu_{max} - D}$$

$$x = Y_{x/s}\left(S_0 - \frac{K_S D}{\mu_{max} - D}\right)$$

Optimization of a Continuous Bioreactor

$$S = \frac{K_s \mu}{\mu_{max} - \mu} = \frac{DK_s}{\mu_{max} - D}$$

$$x = Y_{x/s}\left(S_0 - \frac{K_S D}{\mu_{max} - D}\right)$$

If D is too high, the cells cannot grow fast enough to reach steady state. Then washout will occur.

So maximum dilution rate D_{max} can be found by using $x = 0$ in $x = Y_{x/s}\left(S_0 - \frac{K_S D}{\mu_{max} - D}\right)$

$$D_{max} = \frac{\mu_{max} S_0}{K_s + S_0}$$

Optimization of a Continuous Bioreactor

Define: $\text{Productivity}, P = \dfrac{\text{biomass}}{(\text{reactor volume})\text{time}} = xD$

What should be the optimal dilution rate that will maximize the productivity?

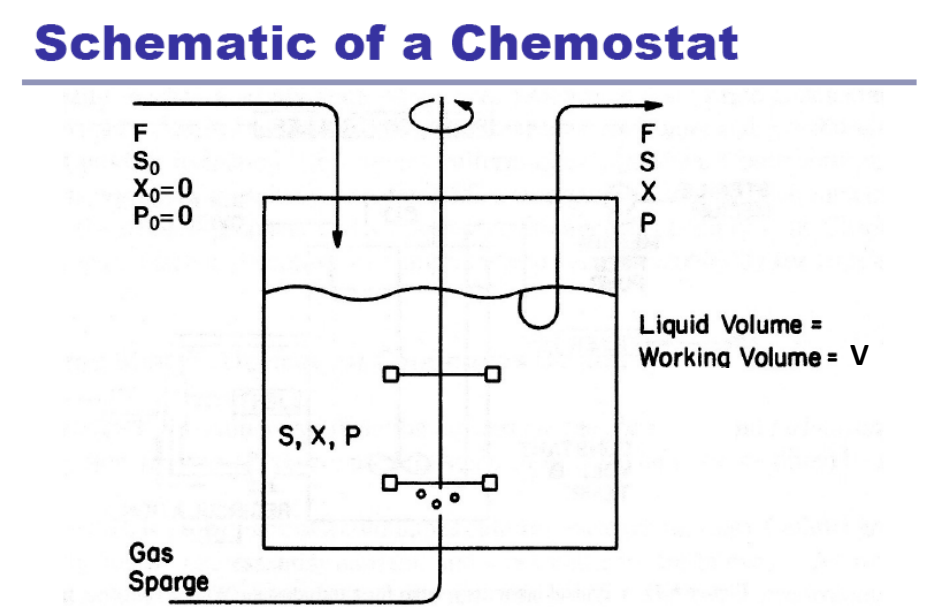
$$\text{Set } \frac{d(xD)}{dD} = 0$$

$$\Rightarrow D_{\text{optimum}} = \mu_{\max}\left(1 - \sqrt{\frac{K_s}{K_s + S_0}}\right)$$

$D_{optimum}$ occurs very close to D_{max}.

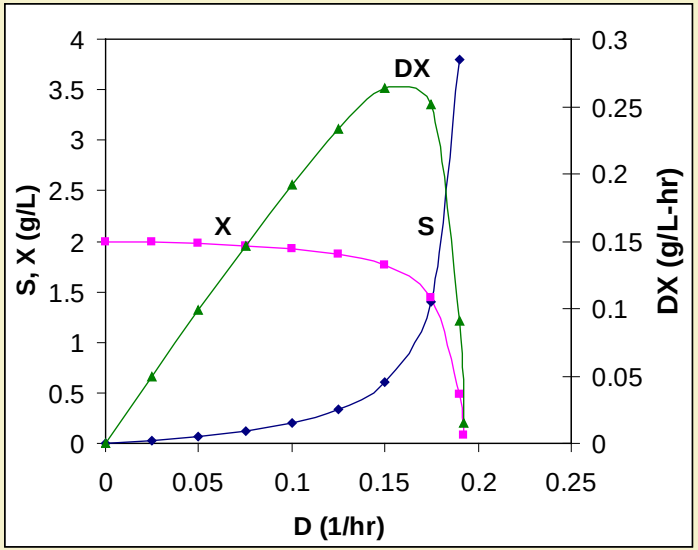
This requires very tight control for successful operation.

Optimization of a Continuous Bioreactor



Productivity = DX

Optimum Productivity = $D_{opt}X_{opt}$



Optimization of a Continuous Bioreactor: Example

$$\frac{dX}{dt} = \mu X - DX$$

$$\frac{dS}{dt} = D(S_0 - S) - \frac{\mu}{Y}X$$

$$\mu = \frac{\mu_{max} S}{K_s + S}$$

$$\mu_{max} = 1\,h^{-1},\ Y_{x/s} = 0.5\,g/g$$

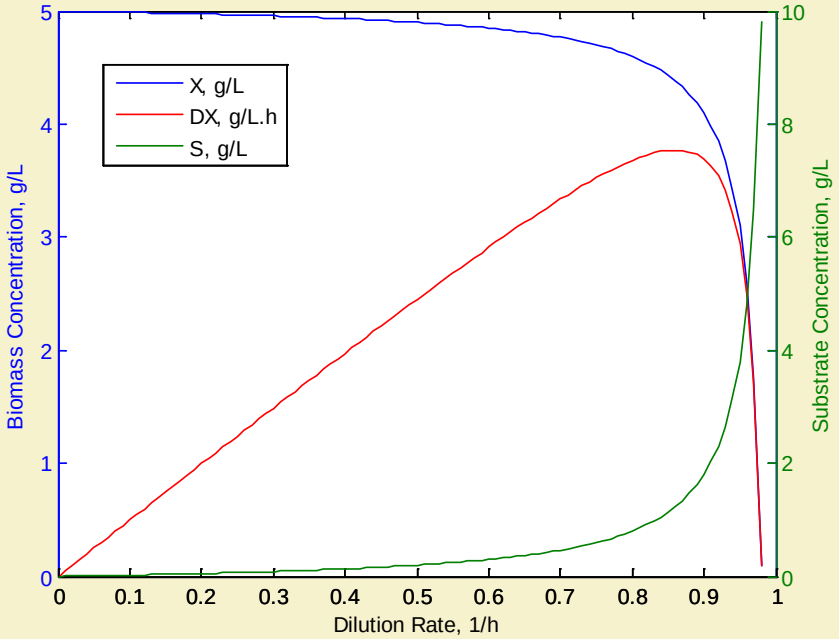
$$K_s = 0.2\,g/L,\ S_0 = 10\,g/L$$

```
mumax = 1;
Yxs = 0.5;
Ks = 0.2;
S0 = 10;
Dmax = mumax*S0/(Ks+S0);
```

```
D = 0:0.01:Dmax;
for i = 1:length(D)
    x(i) = Yxs*(S0 - D(i)*Ks/(mumax-D(i)));
    s(i) = D(i)*Ks/(mumax-D(i));
end
P = D.*x;
```

```
ax = plotyy(D,x, D,s);
ylabel(ax(1), 'Biomass Concentration, g/L');
ylabel(ax(2), 'Substrate Concentration, g/L');
hold on;
plot(D,P, 'r-');
xlabel('Dilution Rate, 1/h');
```

Optimization of a Continuous Bioreactor: Example



D: Dilution rate, h^{-1}

P: Productivity = DX, g/L.h

[D' P']

0.8300	3.7448
0.8400	3.7590
0.8500	3.7683
0.8600	**3.7717**
0.8700	3.7678
0.8800	3.7547

D_{max} = 0.9804

MATLAB Function fminbnd : Example

First write a function file to evaluate objective function:

```
function P = Bior_fminbnd(D)
mumax = 1;
Yxs = 0.5;
Ks = 0.2;
S0 = 10;
x = Yxs*(S0 - Ks*D/(mumax-D));
P = -x*D;
end
```

Now call the optimization solver:

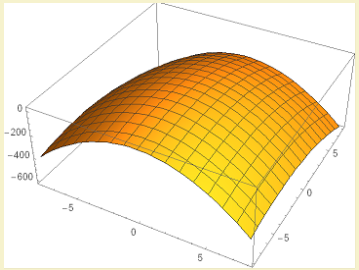
```
options = optimset('Display','iter'); % Option to display output
[x, fval] = fminbnd(@Bior_fminbnd,0,0.98,options)
```

MATLAB Function fminbnd : Example

Func-count	x	f(x)	Procedure
1	0.374327	-1.84924	initial
2	0.605673	-2.93534	golden
3	0.748653	-3.52028	golden
4	0.83702	-3.75523	golden
5	0.891633	-3.72454	golden
6	0.851852	-3.76944	parabolic
7	0.856974	-3.77139	parabolic
8	0.860984	-3.77168	parabolic
9	0.860018	-3.77171	parabolic
10	0.859961	-3.77171	parabolic
11	0.859927	-3.77171	parabolic

```
Optimization terminated:
the current x satisfies the termination criteria using OPTIONS.TolX of 1.000000e-04

x =  0.8600
fval = -3.7717
```

Optimization in Chemical Engineering



Thank You