Equilibrium Extent of Reaction

Contents

Version One. Plot and estimate a solution.

Teaching points of this demonstration:

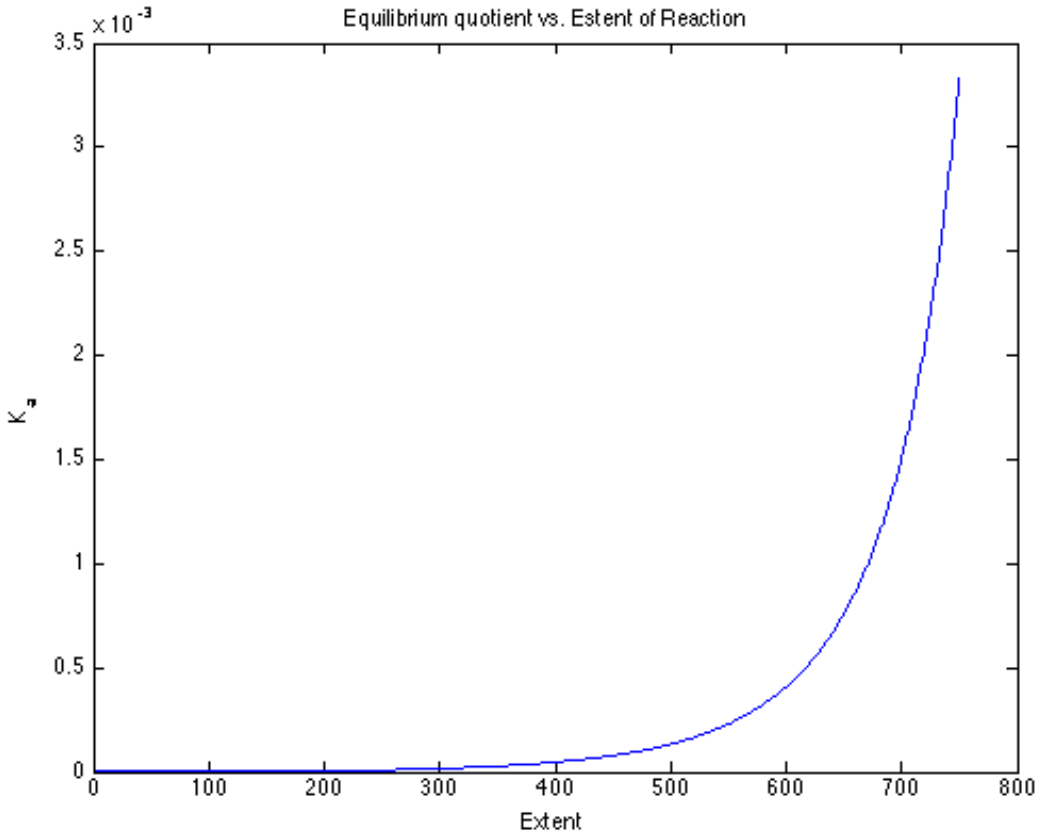
- Use of an anonymous function.
- Use of arrayfun to evaluate a function over a range of values.
- Use of fzero

Create an anonymous function for the equilibrium quotient

```
P = 200;
Ka = @(x) ((2*x)^2 * (4000-2*x)^2) / ((1000 - x)*(3000-3*x)^3*P^2);
```

Create a plot using arrayfun

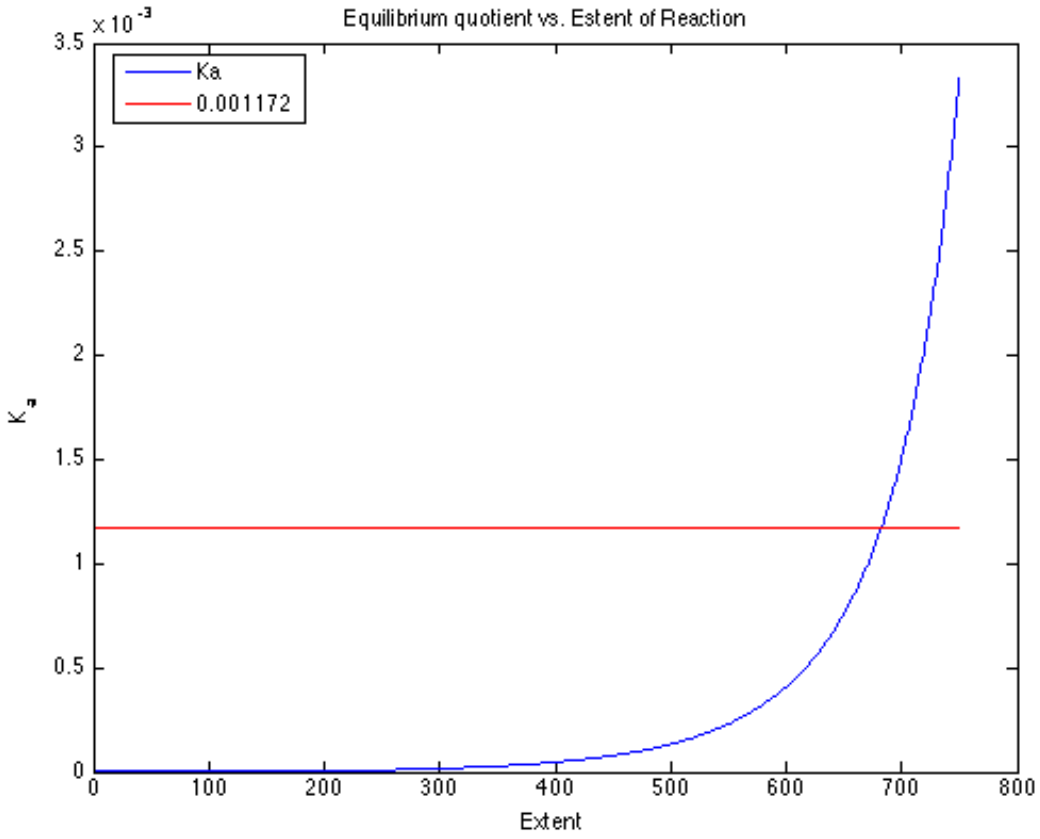
```
figure(1);

x = 0:750;
plot(x,arrayfun(Ka,x));
title('Equilibrium quotient vs. Estent of Reaction');
xlabel('Extent');
ylabel('K_a');
```



Estimate a solution from the plot

Plot the value 0.001172

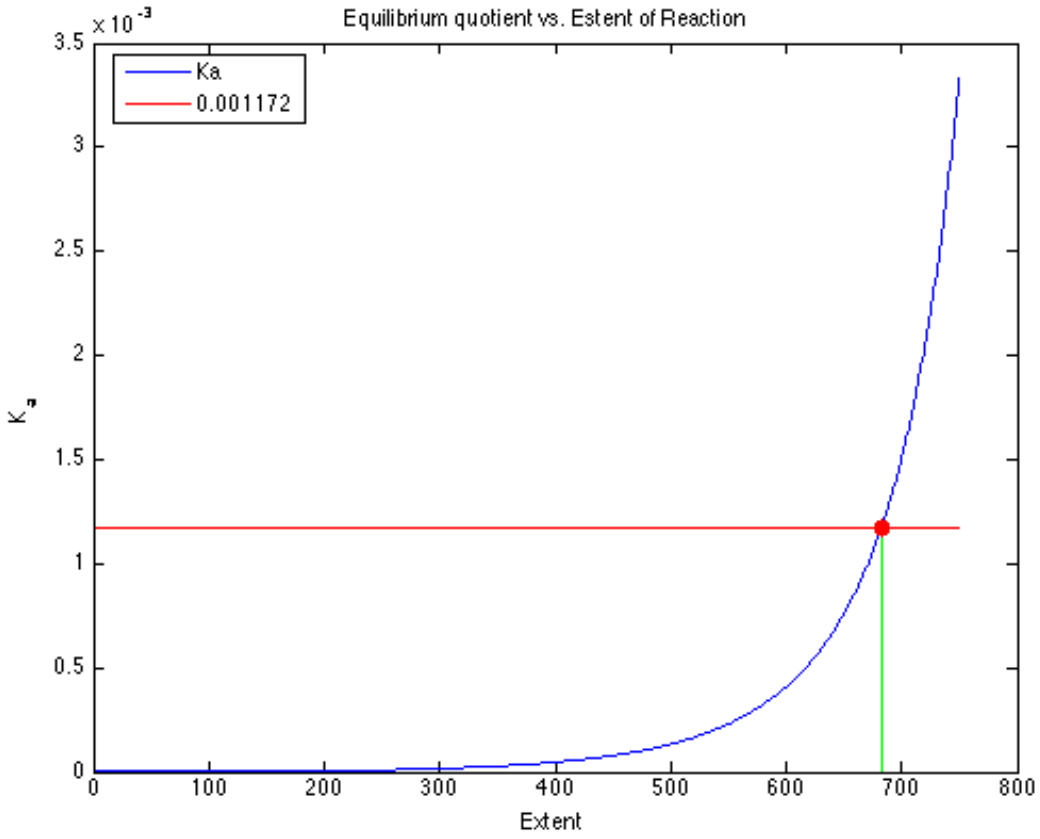
```
hold on;
plot(x,0.001172,'r');
hold off;
legend('Ka','0.001172','location','best');
```



Find a solution using fzero

```
f = @(x) Ka(x) - 0.001172;
xsoln = fzero(f,[0, 999]);

hold on;
plot([xsoln,xsoln],[0 0.001172],'g');
plot(xsoln,0.001172,'r.','Markersize',25);
hold off;
disp(['Equilibrium Extent of Reaction = ',num2str(xsoln),' kgmol/hr']);
```

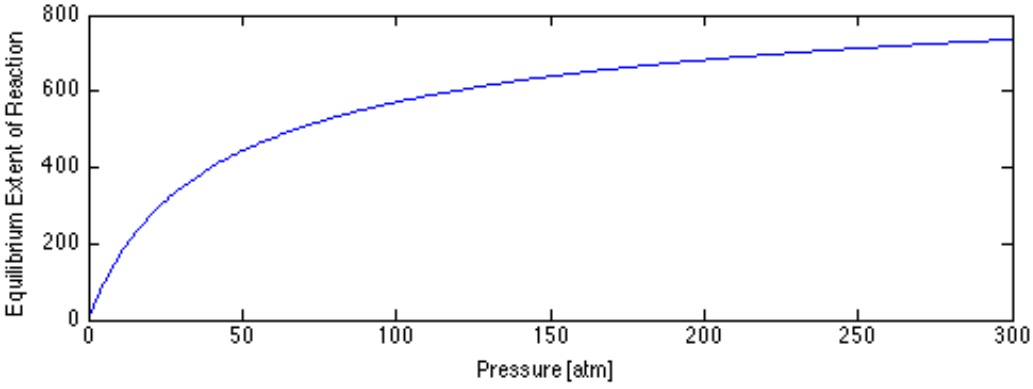
```
Equilibrium Extent of Reaction = 682.0889 kgmol/hr
```

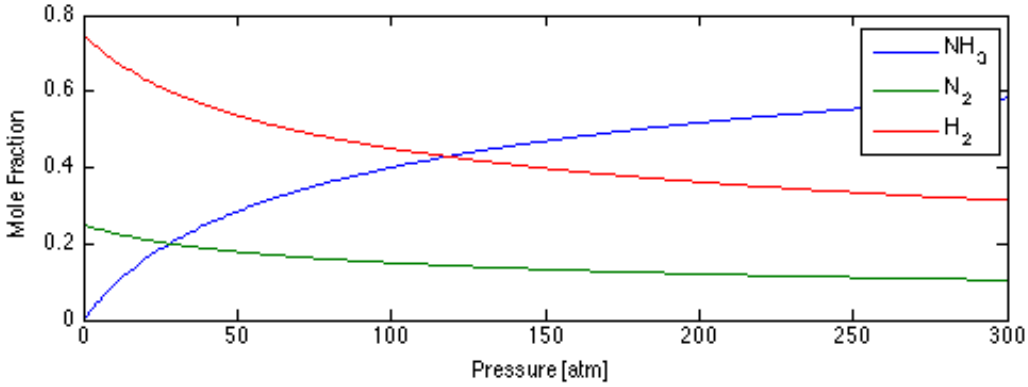


A more elaborate model.

```
% Molar flowrates

nN = @(x) 1000 - x;
nH = @(x) 3000 - 3*x;
nA = @(x) 2*x;

nT = @(x) nN(x) + nH(x) + nA(x);

% Mole fractions

yN = @(x) nN(x)/nT(x);
yH = @(x) nH(x)/nT(x);
yA = @(x) nA(x)/nT(x);

% Equlibrium Extent of Reaction

Ka = @(P,x) (yA(x)^2)/(yN(x)*yH(x)^3*P^2);
x = @(P) fzero(@(x) Ka(P,x) - 0.001172 ,[0,999]);

figure(2);
p = 1:300;
xsoln = arrayfun(x,p);

subplot(2,1,1);
plot(p,xsoln);
xlabel('Pressure [atm]');
ylabel('Equilibrium Extent of Reaction');
```

```
subplot(2,1,2);
plot(p,arrayfun(yA,xsoln),p,arrayfun(yN,xsoln),p,arrayfun(yH,xsoln));
legend('NH_3','N_2','H_2');
xlabel('Pressure [atm]');
ylabel('Mole Fraction');
```





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