
HW5b Equilibrium Concentrations with Two Reactions

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CHEN 3600 - Computer-Aided Chemical Engineering
Spring 2012

```
clear; clc; format short g;
xguess=[3, 3];           % assume 3 moles C from each equation
opts=optimset('TolFun',1e-30, 'TolX', 1e-10);
[soln, resids]=fsolve(@TwoEqxns,xguess,opts);
resids                % note fsolve returns the residuals automatically
soln                  % did not really need to calc them as in my function
[~,concs]=TwoEqxns(soln); % skipping over the resids
concs
```

Equation solved, inaccuracy possible.

The vector of function values is near zero, as measured by the selected value of the function tolerance. However, the last step was ineffective.

resids =

-5.421e-020 -1.3878e-017

soln =

3.3366 2.6772

concs =

40.65 16.663 11.014 7.3228

Referenced External Functions

```
%{
function [ F C ] = TwoEqxns( X )
% TwoEqxns Equation set for HW5b
% Component Locations: A=1, B=2, C=3, D=4
% Note: the source of this problem was rather sloppy with the lack of
% units. Not a chemical engineer! Assume the concentration has units
% of moles.

C0=[50,20,5,10]; % initial concentrations
x1 = X(1); % unpack data
x2 = X(2);
K1eq = 4e-4; % equilibrium constants
K2eq = 3.7e-2;
% establish concentrations at equilibrium
ca = C0(1)-2*x1-x2; % x1 = moles of C formed via first equation
```

```
cb = C0(2)-x1;           % x2 = moles of C formed via second equation
cc = C0(3)+x1+x2;       % note: the source of this problem was rather
cd = C0(4)-x2;
f1 = cc/(ca^2*cb)-K1eq; % calculate target functions to force to zero
f2 = cc/(ca*cd)-K2eq;
F = [f1 f2];            % allow results to be returned
C = [ca cb cc cd];
end
%}
```

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