Matlab array operations vs. matrix operations

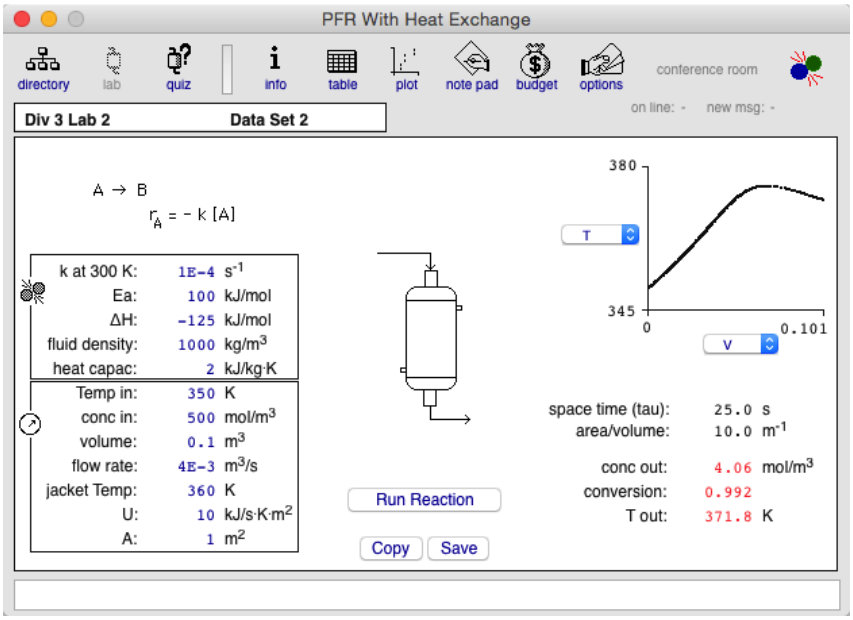
When you are doing an operation involving two arrays (vector or matrix) you have the choice of using two types of operators:
1) array (element-by-element) or "dot" operators, e.g., .* ./
2) matrix (linear algebra) operators (no dot), e.g., * /

When you do an operation involving a scalar (one value) and an array, you can use either type of operator.

For array operations, both arrays must be of the same size: same number rows and same number columns. For matrix operations, the two arrays must be of the size required by the operation. For matrix multiplication, the number of columns of the first array must equal the number of rows of the second array.

Which operator you choose depends on what you are doing. When you are processing experimental data and computing values from the data, you often want to be doing array operations (element-by-element). When you are doing linear algebra, e.g., solving multiple, coupled linear algebraic equations, you want to do matrix operations.

I first discussed an example of doing array operations. In the Reactor Lab, which you can get at www.ReactorLab.net, I copied some data from an experiment with an exothermic reaction in a plug flow reactor with cooling.



I clicked the Copy button and copied the data to the computer clipboard, then pasted it into a Matlab file, which I named today.m. I commented-out the header info. The data are four columns of tab-delimited data.

Editor - /Users/richardherz/Documents/MATLAB/today.m

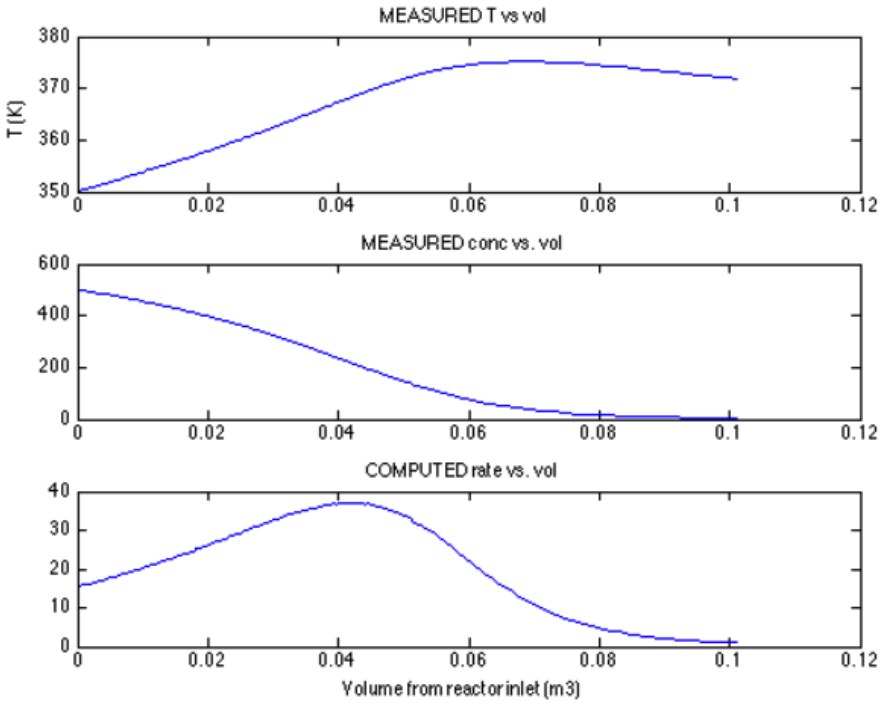
today.m

```
% D3L2 PFR, Data Set 1
%
% k*_1 remained constant at    1.00E-4  1/s (value at 300 K)
% Ea_1 remained constant at      100.0  kJ/mol
% del_H_1 remained constant at    -125.0  kJ/mol
% dens_1 remained constant at       1000  kg/m3
% capac_1 remained constant at       2.00  kJ/(kg K)
% Tin_1 remained constant at      350.0  K
% Cin_1 remained constant at        500  mol/m3
% vol_1 remained constant at      0.100  m3
% flow_1 remained constant at    4.00E-3  m3/s
% Tj_1 remained constant at      360.0  K
% U_1 remained constant at       10.0  kJ/(s K m2)
% A_1 remained constant at       1.00  m2
% tau_1 remained constant at       25.0  s
% V_1 has units of m3
% C_1 has units of mol/m3
% conv_1 has units of (dimensionless)
% T_1 has units of K
%
% V_1   C_1    conv_1      T_1
0   500 0   350.0
5.00E-4 498.1   3.87E-3 350.2
1.00E-3 496.1   7.79E-3 350.4
1.50E-3 494.1   1.18E-2 350.5
2.00E-3 492.1   1.58E-2 350.7
```

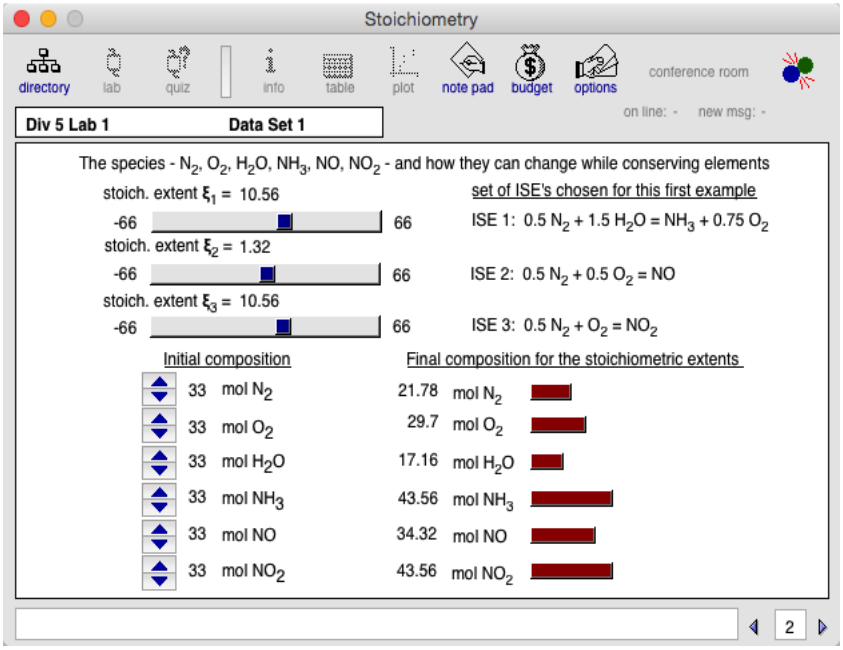
Command Window

Then I wrote a Matlab script which loaded the data file, then computed the rate of reaction at each location in the reactor (volume of reactor from inlet) using array operations.

```
% data from Reactor Lab was saved in file 'today.m'
load 'today.m'

% now have data in array named today
vol = today(:,1);
conc = today(:,2);
T = today(:,4);

subplot(3,1,1), plot(vol,T)
title('MEASURED T vs vol')
ylabel('T (K)')

subplot(3,1,2), plot(vol, conc)
title('MEASURED conc vs. vol')

% now compute reaction rate as a function of vol from reactor inlet
% from measured reactant concentration and T
% rate = k(T)*conc
% k(T) = k(300)*exp(-Ea/Rg * (1/T - 1/300))

% k*_1 remained constant at    1.00E-4  1/s (value at 300 K)
% Ea_1 remained constant at      100.0  kJ/mol

% T is a column vector, so need ./ for array op (element-by-element)
k = 1.00e-4 * exp(-100e3 / 8.3145 * (1 ./ T - 1 / 300));

% k and conc are column vectors, so need .* for array op
rate = k .* conc ;

subplot(3,1,3), plot(vol, rate)
title('COMPUTED rate vs. vol')
xlabel('Volume from reactor inlet (m3)')
```



Next I discussed an example using matrix operations. We looked at a lab in Reactor Lab concerning the stoichiometry of a complex mixture of chemical components which you might encounter in air pollution studies.



With the given list of chemical components, there are three degrees of stoichiometric freedom that allow conservation of the mass of each element. That is, there are three independent stoichiometric equations. An example set of three is shown. For each equation, we can define a "stoichiometric extent" variable, which measures how much each equation has occurred.

Given three stoichmetric equations and three extent values, we use matrix multiplication to compute the change in moles of each chemical component. This is a linear algebra problem involving three simultaneous linear algebraic equations. A Matlab script that solves the example shown above is listed below.

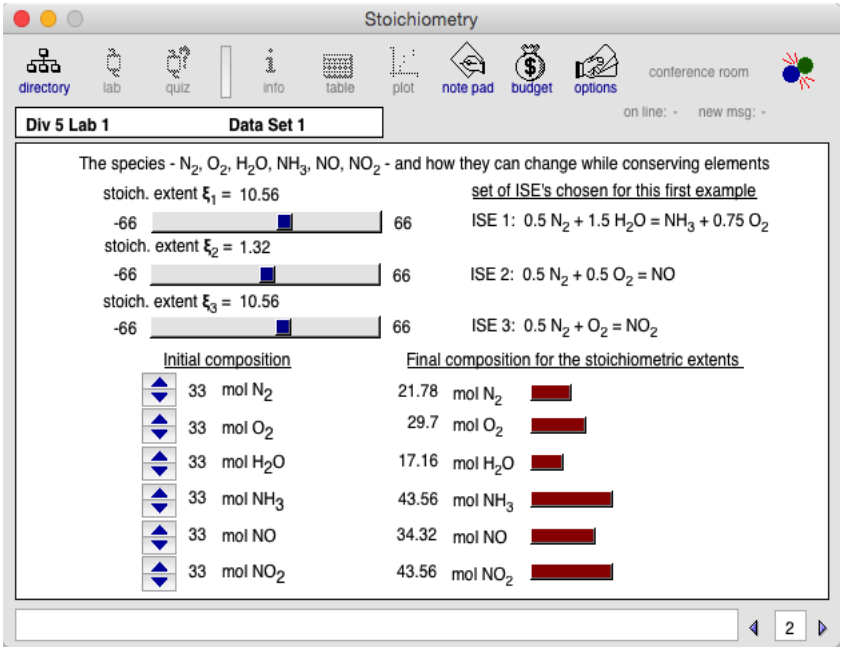
The columns of the matrix Y are the coefficients in the three stoichiometric equations. The rows in Y correspond to the list of chemical components, in the same order as for the columns of matrix A.

```
% List of chemical components present
% N2, O2, H2O, NH3, NO, NO2

% formula matrix
% columns correspond to components in order shown above
% rows correspond to elements
A = [2     0     0     1     1     1   % row -> N
     0     2     1     0     1     2   % row -> O
     0     0     2     3     0     0]; % row -> H

% Y = null(A,'r') % how to get matrix Y in Matlab

% complete stoichiometric matrix
Y = [-0.5000   -0.5000   -0.5000
    0.7500   -0.5000   -1.0000
   -1.5000         0         0
    1.0000         0         0
         0    1.0000         0
         0         0    1.0000];

% for this list of chemical components there are
% three degrees of stoichiometric freedom while
% conserving mass of each element

AY = A*Y % should return null matrix (all zeros)

% initial composition
N0 = [33 33 33 33 33 33]';

e = [10.56 1.32 10.56]'; % example stoichmetric extents

DN = Y*e % vector of change in moles of each component

N = N0 + DN % final moles of each component
```

```
AY =

     0     0     0
     0     0     0
     0     0     0


DN =
```

```
DN =

  -11.2200
   -3.3000
  -15.8400
   10.5600
    1.3200
   10.5600


N =

   21.7800
   29.7000
   17.1600
   43.5600
   34.3200
   43.5600
```

The final N vector computed agrees with the final composition reported by Reactor Lab.



I don't expect you to understand the details of these examples for this course. The purpose here is to show you that both types of operations are useful in engineering.