
Dr. Leon VanDommelen (10/08/19) 3

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IMPORTANT:

Do not change **anything** in this header (besides your name and exam date above as needed)!

Put your solution to the question completely at the end of this file.

EXAM 1, Question 3

```
if ~exist('__code__', 'var') ; clear ; end
format compact
more off
```

Additional file: A2BRates.m

```
function unknownsDerivatives=A2BRates(t,unknowns)

% Function used to compute the concentration changes for
% the reaction
%
%           2 A + B ----> A2B
%
%           unknownsDerivatives=A2BRates(t,unknowns)
%
% Input: t:           time
%         unknowns: concentrations of A, B, and A2B
%
% Output: unknownsDerivatives: the time derivatives of
%                               the unknowns

% take the unknowns out of array unknowns
cA=unknowns(1);
cB=unknowns(2);
cA2B=unknowns(3);

% compute the reaction rate
r=cA^2*cB;

% compute the time derivatives of the unknowns
dcAdt=-2*r;
dcBdt=-r;
dcA2Bdt=r;
```

```
% return them as a column vector
unknownsDerivatives=[dcAdt dcBdt dcA2Bdt]';

end
```

SOLUTION:

```
% show that help works
help A2BRates

% Set the initial conditions
cA0=.25;
cB0=.25;
cA2B0=0;

% set the desired time values
tDesired=linspace(0,100,101);

% solve the system
[tValues, unknownsValues]=ode45(...
    @A2BRates,tDesired,[cA0,cB0,cA2B0]');
cAValues=unknownsValues(:,1);
cBValues=unknownsValues(:,2);
cA2BValues=unknownsValues(:,3);

% plot the solution
plot(tValues,cAValues,'r',...
     tValues,cBValues,'b',...
     tValues,cA2BValues,'k')
```

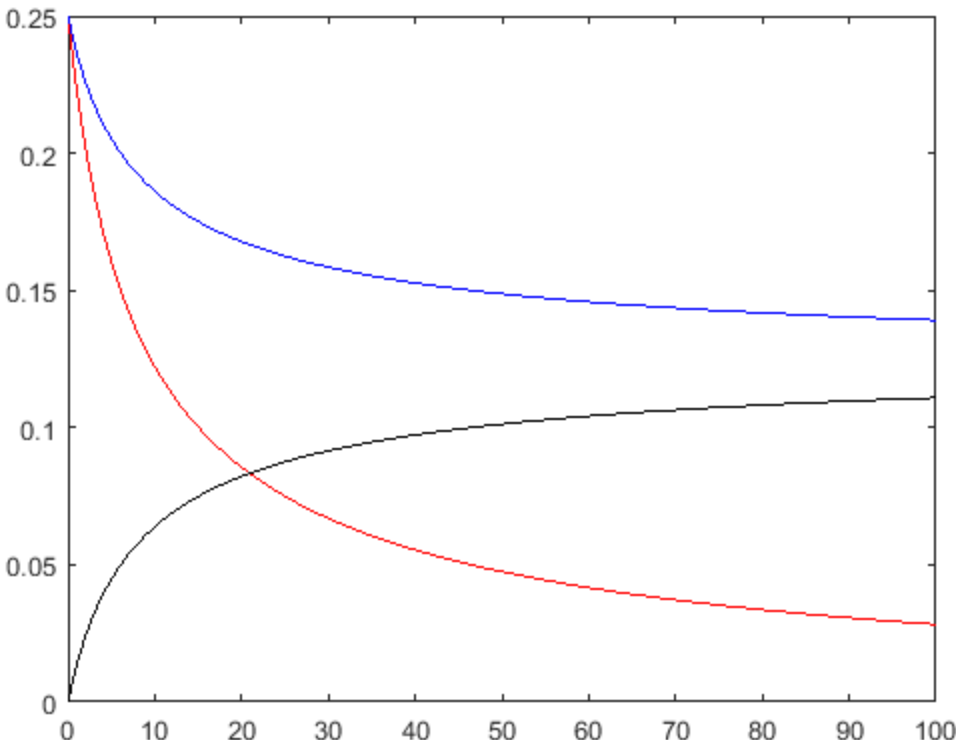
Function used to compute the concentration changes for the reaction

$$2 A + B \text{ ---> } A_2B$$

unknownsDerivatives=A2BRates(t,unknowns)

Input: t: time
unknowns: concentrations of A, B, and A2B

Output: unknownsDerivatives: the time derivatives of the unknowns



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