

# Decomposition of Butadiene

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This is a Matlab script to analyze butadiene decomposition data.

The times at which concentration data was taken are

```
times = [0,1000,1800,2800,3600,4400,5200,6200];
```

The concentration data (moles per liter) is

```
data = [0.01,0.00625,0.00476,0.0037,0.00313,0.0027,0.00241,0.00208];
```

Compute the number of data points

```
N = length(data);
```

Here is a plot of the raw data

```
figure(1)
plot(times, data, '.r', 'MarkerSize', 20);
xlabel("Time (seconds)");
ylabel("Concentration (moles/liter)");
```

Could it be first order?. Perform a logarithmic transformation of the data and plot

```
log_of_data = log(data);
figure(2)
plot(times, log_of_data, '.r', 'MarkerSize', 20);
xlabel("Time (seconds)");
ylabel("log(concentration) (moles/liter)");
```

This is not a straight line, so this is not first order. Still, fit a line and see how it looks

```
c = polyfit(times, log_of_data, 1);
```

Evaluate line at "times", plot with log data

```
fittimes = polyval(c, times);
figure(3)
plot(times, log_of_data, '.r', 'MarkerSize', 20);
hold on
plot(times, fittimes, '-b');
xlabel("Time (seconds)");
ylabel("log(concentration) (moles/liter)");
hold off
```

Perhaps it's second order...