

CHAPTER 1

1.1. For the thermal cracking of ethane in a tubular reactor, the following data were obtained for the rate coefficient at different reference temperatures:

T(°C)	702	725	734	754	773	789	803	810	827	837
k(s ⁻¹)	0.15	0.273	0.333	0.595	0.923	1.492	2.138	2.718	4.137	4.665

Solution

The Arrhenius expression

$$k = A \exp\left(-\frac{E}{RT}\right)$$

is transformed logarithmically into:

$$\ln k = \ln A - \frac{E}{RT}$$

For each data point $\ln k$ and $1/T$ is calculated:

$x = 1/T \cdot 10^3$	$y = \ln k$
1.025	-1.897
1.002	-1.298
0.993	-1.100
0.974	-0.519
0.956	0.080
0.941	0.400
0.929	0.760
0.923	1.000
0.909	1.420
0.901	1.540

The slope and the intercept ($\ln A$) are calculated by linear regression:

$$\frac{E}{R} = \frac{\sum xy - \frac{\sum x \sum y}{N}}{\sum x^2 - \frac{(\sum x)^2}{N}}$$

$$\ln A = \frac{\sum y - m \sum x}{N}$$

with $x = 1/T$ and $y = \ln k$.

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