

## 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 <sup>-1</sup> ) | 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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