

07.02

Trapezoidal Rule for Integration-More Examples Chemical Engineering

Example 1

In an attempt to understand the mechanism of the depolarization process in a fuel cell, an electro-kinetic model for mixed oxygen-methanol current on platinum was developed in the laboratory at FAMU. A very simplified model of the reaction developed suggests a functional relation in an integral form. To find the time required for 50% of the oxygen to be consumed, the time, $T(s)$ is given by

$$T = -\int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx$$

- Use single segment Trapezoidal rule to find the time required for 50% of the oxygen to be consumed.
- Find the true error, E_t , for part (a).
- Find the absolute relative true error, $|\epsilon_t|$, for part (a).

Solution

a) $I \approx (b - a) \left[\frac{f(a) + f(b)}{2} \right]$, where

$$a = 1.22 \times 10^{-6}$$

$$b = 0.61 \times 10^{-6}$$

$$f(x) = -\left[\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right]$$

$$f(1.22 \times 10^{-6}) = -\left[\frac{6.73(1.22 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} (1.22 \times 10^{-6})} \right] = -3.0581 \times 10^{11}$$

$$f(0.61 \times 10^{-6}) = -\left[\frac{6.73(0.61 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} (0.61 \times 10^{-6})} \right] = -3.2104 \times 10^{11}$$

$$I = (0.61 \times 10^{-6} - 1.22 \times 10^{-6}) \left[\frac{-3.0582 \times 10^{11} + (-3.2104 \times 10^{11})}{2} \right]$$

$$= 1.9119 \times 10^5 \text{ s}$$

b) The exact value of the above integral is,

$$T = -\int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx$$

$$= 1.9014 \times 10^5 \text{ s}$$

so the true error is

$$E_t = \text{True Value} - \text{Approximate Value}$$

$$= 1.9014 \times 10^5 - 1.9119 \times 10^5$$

$$= -1056.2$$

c) The absolute relative true error, $|\epsilon_t|$, would then be

$$|\epsilon_t| = \left| \frac{\text{True Error}}{\text{True Value}} \right| \times 100$$

$$= \left| \frac{-1056.2}{1.9014 \times 10^5} \right| \times 100$$

$$= 0.55549 \%$$

Example 2

In an attempt to understand the mechanism of the depolarization process in a fuel cell, an electro-kinetic model for mixed oxygen-methanol current on platinum was developed in the laboratory at FAMU. A very simplified model of the reaction developed suggests a functional relation in an integral form. To find the time required for 50% of the oxygen to be consumed, the time, $T(s)$ is given by

$$T = -\int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx$$

- Use two-segment Trapezoidal rule to find the time required for 50% of the oxygen to be consumed.
- Find the true error, E_t , for part (a).
- Find the absolute relative true error, $|\epsilon_t|$, for part (a).

Solution

$$a) \quad I = \frac{b-a}{2n} \left[f(a) + 2 \left\{ \sum_{i=1}^{n-1} f(a+ih) \right\} + f(b) \right]$$

$$n = 2$$

$$a = 1.22 \times 10^{-6}$$

$$b = 0.61 \times 10^{-6}$$

$$f(x) = - \left[\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right]$$

$$\begin{aligned}
 h &= \frac{b-a}{n} \\
 &= \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2} \\
 &= -0.30500 \times 10^{-6} \\
 f(x_0) &= f(1.22 \times 10^{-6}) \\
 f(1.22 \times 10^{-6}) &= -\left[\frac{6.73(1.22 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(1.22 \times 10^{-6})} \right] = -3.0581 \times 10^{11} \\
 f(x_1) &= f(1.22 \times 10^{-6} - 0.30500 \times 10^{-6}) \\
 &= f(0.91500 \times 10^{-6}) \\
 f(0.91500) &= -\left[\frac{6.73(0.915 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(0.915 \times 10^{-6})} \right] = -3.1089 \times 10^{11} \\
 f(x_2) &= f(x_n) = f(0.61 \times 10^{-6}) \\
 f(0.61 \times 10^{-6}) &= -\left[\frac{6.73(0.61 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(0.61 \times 10^{-6})} \right] = -3.2104 \times 10^{11} \\
 I &= \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2(2)} \left[f(1.22 \times 10^{-6}) + 2 \left\{ \sum_{i=1}^{2-1} f(a+ih) \right\} + f(0.61 \times 10^{-6}) \right] \\
 &= \frac{-0.61 \times 10^{-6}}{4} \left[f(1.22 \times 10^{-6}) + 2f(0.915 \times 10^{-6}) + f(0.61 \times 10^{-6}) \right] \\
 &= \frac{-0.61 \times 10^{-6}}{4} \left[-3.0581 \times 10^{11} + 2(-3.1089 \times 10^{11}) - 3.2104 \times 10^{11} \right] \\
 &= 1.9042 \times 10^5 \text{ s}
 \end{aligned}$$

b) The exact value of the above integral is,

$$\begin{aligned}
 T &= -\int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx \\
 &= 1.90140 \times 10^5 \text{ s}
 \end{aligned}$$

so the true error is

$$\begin{aligned}
 E_t &= \text{True Value} - \text{Approximate Value} \\
 &= 1.90140 \times 10^5 - 1.9042 \times 10^5 \\
 &= -282.12
 \end{aligned}$$

c) The absolute relative true error, $|\epsilon_t|$, would then be

$$\begin{aligned}
 |\epsilon_t| &= \left| \frac{\text{True Error}}{\text{True Value}} \right| \times 100 \\
 &= \left| \frac{-282.12}{1.9014 \times 10^5} \right| \times 100 \\
 &= 0.14838 \%
 \end{aligned}$$

Table 1 Values obtained using multiple-segment Trapezoidal rule for

$$T = -\int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx$$

n	Value	E_t	$ \epsilon_t \%$	$ \epsilon_a \%$
1	191190	-1056.2	0.55549	---
2	190420	-282.12	0.14838	0.40711
3	190260	-127.31	0.066956	0.081424
4	190210	-72.017	0.037877	0.029079
5	190180	-46.216	0.024307	0.013570
6	190170	-32.142	0.016905	0.0074020
7	190160	-23.636	0.012431	0.0044740
8	190150	-18.107	0.0095231	0.0029079