

07.03

Simpson's 1/3 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 Simpson's 1/3 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

$$a) \quad T \approx \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

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

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

$$\frac{a+b}{2} = 0.91500 \times 10^{-6}$$

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

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

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

$$\begin{aligned}
 f(0.91500 \times 10^{-6}) &= -\left[\frac{6.73(0.91500 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(0.91500 \times 10^{-6})} \right] = -3.1089 \times 10^{11} \\
 T &= \left(\frac{b-a}{6} \right) \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right] \\
 &= \left(\frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{6} \right) \left[f(1.22 \times 10^{-6}) + 4f(0.915 \times 10^{-6}) + f(0.61 \times 10^{-6}) \right] \\
 &= \left(\frac{-0.61 \times 10^{-6}}{6} \right) \left[-3.0581 \times 10^{11} + 4(-3.1089 \times 10^{11}) - 3.2104 \times 10^{11} \right] \\
 &= 190160 \text{ s}
 \end{aligned}$$

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

$$\begin{aligned}
 E_t &= \text{True Value} - \text{Approximate Value} \\
 &= 1.90140 \times 10^5 - 190160 \\
 &= -24.100
 \end{aligned}$$

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

$$\begin{aligned}
 |\epsilon_t| &= \left| \frac{\text{True Error}}{\text{True Value}} \right| \times 100 \\
 &= \left| \frac{-24.020}{1.90140 \times 10^5} \right| \times 100 \\
 &= 0.012675 \%
 \end{aligned}$$

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

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

a) Use four-Simpson's 1/3 Rule to find the time required for 50% of the oxygen to be consumed.

- b) Find the true error, E_t , for part (a).
 c) Find the absolute relative true error, $|\epsilon_t|$, for part (a).

Solution

$$a) \quad T = \frac{b-a}{3n} \left[f(x_0) + 4 \sum_{\substack{i=1 \\ i=odd}}^{n-1} f(x_i) + 2 \sum_{\substack{i=2 \\ i=even}}^{n-2} f(x_i) + f(x_n) \right]$$

$$n = 4$$

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

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

$$h = \frac{b-a}{n}$$

$$= \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{4}$$

$$= -0.15250 \times 10^{-6}$$

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

So

$$f(x_0) = f(1.22 \times 10^{-6})$$

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

$$f(x_1) = f(1.22 \times 10^{-6} - 0.15250 \times 10^{-6}) = f(1.0675 \times 10^{-6})$$

$$f(1.0675 \times 10^{-6}) = - \left[\frac{6.73(1.0675 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} (1.0675 \times 10^{-6})} \right] = -3.0799 \times 10^{11}$$

$$f(x_2) = f(1.0675 \times 10^{-6} - 0.15250 \times 10^{-6}) = f(0.915 \times 10^{-6})$$

$$f(0.915 \times 10^{-6}) = - \left[\frac{6.73(0.915 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} (0.915 \times 10^{-6})} \right] = -3.1089 \times 10^{11}$$

$$f(x_3) = f(0.915 \times 10^{-6} - 0.15250 \times 10^{-6}) = f(0.76250 \times 10^{-6})$$

$$f(0.76250 \times 10^{-6}) = - \left[\frac{6.73(0.76250 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} (0.76250 \times 10^{-6})} \right] = -3.1495 \times 10^{11}$$

$$f(x_4) = f(x_n) = f(0.61 \times 10^{-6})$$

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

$$\begin{aligned}
T &= \frac{b-a}{3n} \left[f(x_0) + 4 \sum_{\substack{i=1 \\ i=\text{odd}}}^{n-1} f(x_i) + 2 \sum_{\substack{i=2 \\ i=\text{even}}}^{n-2} f(x_i) + f(x_n) \right] \\
&= \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{3(4)} \left[f(1.22 \times 10^{-6}) + 4 \sum_{\substack{i=1 \\ i=\text{odd}}}^3 f(x_i) \right. \\
&\quad \left. + 2 \sum_{\substack{i=2 \\ i=\text{even}}}^2 f(x_i) + f(0.61 \times 10^{-6}) \right] \\
&= \frac{-0.61 \times 10^{-6}}{12} [f(1.22 \times 10^{-6}) + 4f(x_1) + 4f(x_3) + 2f(x_2) + f(0.61 \times 10^{-6})] \\
&= \frac{-0.61 \times 10^{-6}}{12} [f(1.22 \times 10^{-6}) + 4f(1.0675 \times 10^{-6}) + \\
&\quad 4f(0.76250 \times 10^{-6}) + 2f(0.915 \times 10^{-6}) + f(0.61 \times 10^{-6})] \\
&= \frac{-0.61 \times 10^{-6}}{12} [-3.0582 \times 10^{11} + 4(-3.0799 \times 10^{11}) + \\
&\quad 4(-3.1495 \times 10^{11}) + 2(-3.1089 \times 10^{11}) - 3.2104 \times 10^{11}] \\
&= 190140 \text{ s}
\end{aligned}$$

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

$$\begin{aligned}
E_t &= \text{True Value} - \text{Approximate Value} \\
&= 1.90140 \times 10^5 - 190140 \\
&= -1.9838
\end{aligned}$$

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

$$\begin{aligned}
|\epsilon_t| &= \left| \frac{\text{True Error}}{\text{True Value}} \right| \times 100 \\
&= \left| \frac{-1.9838}{1.90140 \times 10^5} \right| \times 100 \\
&= 0.0010434 \%
\end{aligned}$$

Table 1 Values of Simpson's 1/3 Rule for Example 2 with multiple segments.

n	Approximate Value	E_t	$ \epsilon_t $ %
2	190160	-24.100	0.012675
4	190140	-1.9838	0.0010434
6	190140	-0.42010	2.2094×10^{-4}
8	190140	-0.13655	7.1815×10^{-5}
10	190140	-0.056663	2.9802×10^{-5}