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

$$T = -\int_{1.22\times10^{-6}}^{0.61\times10^{-6}} \left(\frac{6.73x + 4.3025\times10^{-7}}{2.316\times10^{-11}x} \right) dx$$

a) Use 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, $|\in_t|$, for part (a).

Solution

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

$$a = 1.22\times10^{-6}$$

$$b = 0.61\times10^{-6}$$

$$\frac{a+b}{2} = 0.91500\times10^{-6}$$

$$f(x) = -\left[\frac{6.73x + 4.3025\times10^{-7}}{2.316\times10^{-11}x} \right]$$

$$f\left(1.22\times10^{-6}\right) = -\left[\frac{6.73\left(1.22\times10^{-6}\right) + 4.3025\times10^{-7}}{2.316\times10^{-11}\left(1.22\times10^{-6}\right)} \right] = -3.0581\times10^{11}$$

$$f\left(0.61\times10^{-6}\right) = -\left[\frac{6.73\left(0.61\times10^{-6}\right) + 4.3025\times10^{-7}}{2.316\times10^{-11}\left(0.61\times10^{-6}\right)} \right] = -3.2104\times10^{11}$$

$$f\left(0.91500\times10^{-6}\right)=-\left[\frac{6.73\left(0.91500\times10^{-6}\right)+4.3025\times10^{-7}}{2.316\times10^{-11}\left(0.91500\times10^{-6}\right)}\right]=-3.1089\times10^{11}$$

$$\begin{aligned}
T &= \left(\frac{b-a}{6}\right)\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]\\
&= \left(\frac{0.61\times10^{-6}-1.22\times10^{-6}}{6}\right)\left[f\left(1.22\times10^{-6}\right)+4f\left(0.915\times10^{-6}\right)+f\left(0.61\times10^{-6}\right)\right]\\
&= \left(\frac{-0.61\times10^{-6}}{6}\right)\left[-3.0581\times10^{11}+4\left(-3.1089\times10^{11}\right)-3.2104\times10^{11}\right]\\
&= 190160 \text{ s}
\end{aligned}$$

b) The exact value of the above integral is,

$$T=-\int_{1.22\times10^{-6}}^{0.61\times10^{-6}}\left(\frac{6.73x+4.3025\times10^{-7}}{2.316\times10^{-11}x}\right)dx$$

$$=1.90140\times10^{5}\text{s}$$

so the true error is

$$\begin{aligned}
E_t &= \textit{True Value} - \textit{Approximate Value}\\
&= 1.90140\times10^{5}-190160\\
&= -24.100
\end{aligned}$$

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

$$\begin{aligned}
|\in_t| &= \left|\frac{\text{True Error}}{\text{True Value}}\right|\times100\\
&= \left|\frac{-24.020}{1.90140\times10^{5}}\right|\times100\\
&= 0.012675\,\%
\end{aligned}$$

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

$$T=-\int_{1.22\times10^{-6}}^{0.61\times10^{-6}}\left(\frac{6.73x+4.3025\times10^{-7}}{2.316\times10^{-11}x}\right)dx$$

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, $|\in_t|$, for part (a).

Solution

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

$$n = 4$$
$$a = 1.22\times10^{-6}$$
$$b = 0.61\times10^{-6}$$
$$h = \frac{b-a}{n}$$
$$= \frac{0.61\times10^{-6} - 1.22\times10^{-6}}{4}$$
$$= -0.15250\times10^{-6}$$
$$f(x) = -\left[\frac{6.73x + 4.3025\times10^{-7}}{2.316\times10^{-11}x}\right]$$

So

$$f(x_0) = f\left(1.22\times10^{-6}\right)$$
$$f\left(1.22\times10^{-6}\right) = -\left[\frac{6.73\left(1.22\times10^{-6}\right) + 4.3025\times10^{-7}}{2.316\times10^{-11}\left(1.22\times10^{-6}\right)}\right] = -3.0581\times10^{11}$$

$$f(x_1) = f\left(1.22\times10^{-6} - 0.15250\times10^{-6}\right) = f\left(1.0675\times10^{-6}\right)$$
$$f\left(1.0675\times10^{-6}\right) = -\left[\frac{6.73\left(1.0675\times10^{-6}\right) + 4.3025\times10^{-7}}{2.316\times10^{-11}\left(1.0675\times10^{-6}\right)}\right] = -3.0799\times10^{11}$$
$$f(x_2) = f\left(1.0675\times10^{-6} - 0.15250\times10^{-6}\right) = f\left(0.915\times10^{-6}\right)$$
$$f\left(0.915\times10^{-6}\right) = -\left[\frac{6.73\left(0.915\times10^{-6}\right) + 4.3025\times10^{-7}}{2.316\times10^{-11}\left(0.915\times10^{-6}\right)}\right] = -3.1089\times10^{11}$$

$$f(x_3) = f\left(0.915\times10^{-6} - 0.15250\times10^{-6}\right) = f\left(0.76250\times10^{-6}\right)$$
$$f\left(0.76250\times10^{-6}\right) = -\left[\frac{6.73\left(0.76250\times10^{-6}\right) + 4.3025\times10^{-7}}{2.316\times10^{-11}\left(0.76250\times10^{-6}\right)}\right] = -3.1495\times10^{11}$$

$$f(x_4) = f(x_n) = f\left(0.61\times10^{-6}\right)$$
$$f\left(0.61\times10^{-6}\right) = -\left[\frac{6.73\left(0.61\times10^{-6}\right) + 4.3025\times10^{-7}}{2.316\times10^{-11}\left(0.61\times10^{-6}\right)}\right] = -3.2104\times10^{11}$$

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

$$= \frac{0.61\times10^{-6} - 1.22\times10^{-6}}{3(4)}\left[\begin{array}{l} f(1.22\times10^{-6}) + 4\sum\limits_{\substack{i=1\\ i=odd}}^{3} f(x_i) \\ + 2\sum\limits_{\substack{i=2\\ i=even}}^{2} f(x_i) + f(0.61\times10^{-6}) \end{array}\right]$$

$$= \frac{-0.61\times10^{-6}}{12}\left[f(1.22\times10^{-6}) + 4f(x_1) + 4f(x_3) + 2f(x_2) + f(0.61\times10^{-6})\right]$$

$$= \frac{-0.61\times10^{-6}}{12}\left[\begin{array}{l} f(1.22\times10^{-6}) + 4f(1.0675\times10^{-6}) + \\ 4f(0.76250\times10^{-6}) + 2f(0.915\times10^{-6}) + f(0.61\times10^{-6}) \end{array}\right]$$

$$= \frac{-0.61\times10^{-6}}{12}\left[\begin{array}{l} -3.0582\times10^{11} + 4(-3.0799\times10^{11}) + \\ 4(-3.1495\times10^{11}) + 2(-3.1089\times10^{11}) - 3.2104\times10^{11} \end{array}\right]$$

$$= 190140 \text{ s}$$

b) The exact value of the above integral is

$$T = -\int_{1.22\times10^{-6}}^{0.61\times10^{-6}}\left(\frac{6.73x + 4.3025\times10^{-7}}{2.316\times10^{-11}x}\right)dx$$

$$= 1.90140\times10^{5} \text{ s}$$

so the true error is

$$E_t = True\ Value - Approximate\ Value$$

$$= 1.90140\times10^{5} - 190140$$

$$= -1.9838$$

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

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

$$= \left|\frac{-1.9838}{1.90140\times10^{5}}\right| \times 100$$

$$= 0.0010434\ \%$$

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

n	Approximate Value	E_t	$\lvert \in_t \rvert$ %
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}