

07.06 Gauss Quadrature 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 two-point Gauss quadrature rule to find the time required for 50 % of the oxygen to be consumed. Also, find the absolute relative true error.

Solution

First, change the limits of integration from $[1.22 \times 10^{-6}, 0.61 \times 10^{-6}]$ to $[-1, 1]$ using

$$\int_a^b f(x) dx = \frac{b-a}{2} \int_{-1}^1 f\left(\frac{b-a}{2}x + \frac{b+a}{2}\right) dx$$

gives

$$\begin{aligned} \int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} f(x) dx &= \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2} \int_{-1}^1 f\left(\frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2}x + \frac{0.61 \times 10^{-6} + 1.22 \times 10^{-6}}{2}\right) dx \\ &= -0.305 \times 10^{-6} \int_{-1}^1 f(-3.05 \times 10^{-6}x + 0.91500 \times 10^{-6}) dx \end{aligned}$$

Next, get weighting factors and function argument values from Table 1 for the two point rule,

$$c_1 = 1.0000$$

$$x_1 = -0.57735$$

$$c_2 = 1.0000$$

$$x_2 = 0.57735$$

Now we can use the Gauss Quadrature formula

$$\begin{aligned}
& -0.305 \times 10^{-6} \int_{-1}^1 f(-0.305 \times 10^{-6} x + 0.915 \times 10^{-6}) dx \\
& \approx -0.305 \times 10^{-6} \left[c_1 f(-0.305 \times 10^{-6} x_1 + 0.915 \times 10^{-6}) \right. \\
& \quad \left. + c_2 f(-0.305 \times 10^{-6} x_2 + 0.915 \times 10^{-6}) \right] \\
& \approx -0.305 \times 10^{-6} \left[f(-0.305 \times 10^{-6}(-0.57735) + 0.915 \times 10^{-6}) \right. \\
& \quad \left. + f(-0.305 \times 10^{-6}(0.57735) + 0.915 \times 10^{-6}) \right] \\
& \approx -0.305 \times 10^{-6} \left[f(1.0911 \times 10^{-6}) + f(0.73891 \times 10^{-6}) \right] \\
& \approx -0.305 \times 10^{-6} \left[(-3.0761 \times 10^{11}) + (-3.1573 \times 10^{11}) \right] \\
& \approx 190120 \text{ s}
\end{aligned}$$

since

$$\begin{aligned}
f(1.0911 \times 10^{-6}) &= - \left[\frac{6.73(1.0911 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(1.0911 \times 10^{-6})} \right] \\
&= -3.0761 \times 10^{11} \\
f(0.73891 \times 10^{-6}) &= - \left[\frac{6.73(0.73891 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(0.73891 \times 10^{-6})} \right] \\
&= -3.1573 \times 10^{11}
\end{aligned}$$

The absolute relative true error, $|\epsilon_t|$, is (Exact value = 190140 s)

$$\begin{aligned}
|\epsilon_t| &= \left| \frac{1.90140 \times 10^5 - 190140}{1.90140 \times 10^5} \right| \times 100 \% \\
&= 0.0082023 \%
\end{aligned}$$

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

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

Use three-point Gauss quadrature rule to find the time required for 50 % of the oxygen to be consumed. Also, find the absolute relative true error.

Solution

First, change the limits of integration from $[1.22 \times 10^{-6}, 0.61 \times 10^{-6}]$ to $[-1, 1]$ using Equation 23 gives

$$\int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} f(x) dx = \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2} \int_{-1}^1 f \left(\frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2} x + \frac{0.61 \times 10^{-6} + 1.22 \times 10^{-6}}{2} \right) dx$$

$$= -0.305 \times 10^{-6} \int_{-1}^1 f(-0.305 \times 10^{-6} x + 0.915 \times 10^{-6}) dx$$

The weighting factors and function argument values are

$$c_1 = 0.55556$$

$$x_1 = -0.77460$$

$$c_2 = 0.88889$$

$$x_2 = 0.0000$$

$$c_3 = 0.55556$$

$$x_3 = 0.77460$$

and the formula is

$$-0.305 \times 10^{-6} \int_{-1}^1 f(-0.305 \times 10^{-6} x + 0.915 \times 10^{-6}) dx$$

$$\approx -0.305 \times 10^{-6} \left[c_1 f(-0.305 \times 10^{-6} x_1 + 0.915 \times 10^{-6}) \right. \\ \left. + c_2 f(-0.305 \times 10^{-6} x_2 + 0.915 \times 10^{-6}) \right. \\ \left. + c_3 f(-0.305 \times 10^{-6} x_3 + 0.915 \times 10^{-6}) \right]$$

$$\approx -0.305 \times 10^{-6} \left[0.55556 f(-0.305 \times 10^{-6} (-0.77456) + 0.915 \times 10^{-6}) \right. \\ \left. + 0.88889 f(-0.305 \times 10^{-6} (0.0000) + 0.915 \times 10^{-6}) \right. \\ \left. + 0.55556 f(-0.305 \times 10^{-6} (0.77456) + 0.915 \times 10^{-6}) \right]$$

$$\approx -0.305 \times 10^{-6} \left[0.55556 f(1.1512 \times 10^{-6}) + 0.88889 f(0.915 \times 10^{-6}) \right. \\ \left. + 0.55556 f(0.67876 \times 10^{-6}) \right]$$

$$\approx -0.305 \times 10^{-6} \left[0.55556 (-3.0673 \times 10^{11}) + 0.88889 (-3.1098 \times 10^{11}) \right. \\ \left. + 0.55556 (-3.1796 \times 10^{11}) \right]$$

$$\approx 190140 \text{ s}$$

since

$$f(1.1512 \times 10^{-6}) = - \left[\frac{6.73(1.1512 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} (1.1512 \times 10^{-6})} \right]$$

$$= -3.0672 \times 10^{11}$$

$$\begin{aligned}f(0.915 \times 10^{-6}) &= -\left[\frac{6.73(0.915 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(0.915 \times 10^{-6})} \right] \\&= -3.1089 \times 10^{11} \\f(0.67876 \times 10^{-6}) &= -\left[\frac{6.73(0.67876 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(0.67876 \times 10^{-6})} \right] \\&= -3.1796 \times 10^{11}\end{aligned}$$

The absolute relative true error, $|\epsilon_t|$, is (Exact value = 190140 s)

$$\begin{aligned}|\epsilon_t| &= \left| \frac{190140 - (190140)}{190140} \right| \times 100\% \\&= 0.00024868 \%\end{aligned}$$