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 $\left[1.22\times 10^{-6},\, 0.61\times 10^{-6}\right]$ 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

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

$$= -0.305\times 10^{-6}\int_{-1}^{1} f\left(-3.05\times 10^{-6}x + 0.91500\times 10^{-6}\right)dx$$

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

$$
\begin{aligned}
&-0.305\times10^{-6}\int_{-1}^{1} f\left(-0.305\times10^{-6}x+0.915\times10^{-6}\right)dx \\
&\approx -0.305\times10^{-6}\begin{bmatrix} c_1 f\left(-0.305\times10^{-6}x_1+0.915\times10^{-6}\right) \\ +c_2 f\left(-0.305\times10^{-6}x_2+0.915\times10^{-6}\right)\end{bmatrix} \\
&\approx -0.305\times10^{-6}\begin{bmatrix} f\left(-0.305\times10^{-6}(-0.57735)+0.915\times10^{-6}\right) \\ +f\left(-0.305\times10^{-6}(0.57735)+0.915\times10^{-6}\right)\end{bmatrix} \\
&\approx -0.305\times10^{-6}\left[f\left(1.0911\times10^{-6}\right)+f\left(0.73891\times10^{-6}\right)\right] \\
&\approx -0.305\times10^{-6}\left[\left(-3.0761\times10^{11}\right)+\left(-3.1573\times10^{11}\right)\right] \\
&\approx 190120 \text{ s}
\end{aligned}
$$

since

$$
\begin{aligned}
f\left(1.0911\times10^{-6}\right) &= -\left[\frac{6.73\left(1.0911\times10^{-6}\right)+4.3025\times10^{-7}}{2.316\times10^{-11}\left(1.0911\times10^{-6}\right)}\right] \\
&= -3.0761\times10^{11} \\
f\left(0.73891\times10^{-6}\right) &= -\left[\frac{6.73\left(0.73891\times10^{-6}\right)+4.3025\times10^{-7}}{2.316\times10^{-11}\left(0.73891\times10^{-6}\right)}\right] \\
&= -3.1573\times10^{11}
\end{aligned}
$$

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

$$
\begin{aligned}
|\in_t| &= \left|\frac{1.90140\times10^{5}-190140}{1.90140\times10^{5}}\right|\times100\,\% \\
&= 0.0082023\,\%
\end{aligned}
$$

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

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

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 $\left[1.22\times10^{-6},\ 0.61\times10^{-6}\right]$ to $[-1,1]$ using Equation 23 gives

$$\int_{1.22\times10^{-6}}^{0.61\times10^{-6}} f(x)dx = \frac{0.61\times10^{-6}-1.22\times10^{-6}}{2}\int_{-1}^{1} f\left(\frac{0.61\times10^{-6}-1.22\times10^{-6}}{2}x + \frac{0.61\times10^{-6}+1.22\times10^{-6}}{2}\right)dx$$

$$= -0.305\times10^{-6}\int_{-1}^{1} f\left(-3.05\times10^{-6}x + 0.915\times10^{-6}\right)dx$$

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

$$-0.305\times10^{-6}\int_{-1}^{1} f\left(-0.305\times10^{-6}x + 0.915\times10^{-6}\right)dx$$

$$\approx -0.305\times10^{-6}\begin{bmatrix} c_1 f\left(-0.305\times10^{-6}x_1 + 0.915\times10^{-6}\right) \\ + c_2 f\left(-0.305\times10^{-6}x_2 + 0.915\times10^{-6}\right) \\ + c_3 f\left(-0.305\times10^{-6}x_3 + 0.915\times10^{-6}\right) \end{bmatrix}$$

$$\approx -0.305\times10^{-6}\begin{bmatrix} 0.55556 f\left(-0.305\times10^{-6}(-0.77456) + 0.915\times10^{-6}\right) \\ + 0.88889 f\left(-0.305\times10^{-6}(0.0000) + 0.915\times10^{-6}\right) \\ + 0.55556 f\left(-0.305\times10^{-6}(0.77456) + 0.915\times10^{-6}\right) \end{bmatrix}$$

$$\approx -0.305\times10^{-6}\begin{bmatrix} 0.55556 f\left(1.1512\times10^{-6}\right) + 0.88889 f\left(0.915\times10^{-6}\right) \\ + 0.55556 f\left(0.67876\times10^{-6}\right) \end{bmatrix}$$

$$\approx -0.305\times10^{-6}\begin{bmatrix} 0.55556\left(-3.0673\times10^{11}\right) + 0.88889\left(-3.1098\times10^{11}\right) \\ + 0.55556\left(-3.1796\times10^{11}\right) \end{bmatrix}$$

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

since

$$f\left(1.1512\times10^{-6}\right) = -\left[\frac{6.73\left(1.1512\times10^{-6}\right) + 4.3025\times10^{-7}}{2.316\times10^{-11}\left(1.1512\times10^{-6}\right)}\right]$$

$$= -3.0672\times10^{11}$$

$$f\left(0.915\times10^{-6}\right)=-\left[\frac{6.73\left(0.915\times10^{-6}\right)+4.3025\times10^{-7}}{2.316\times10^{-11}\left(0.915\times10^{-6}\right)}\right]$$
$$=-3.1089\times10^{11}$$
$$f\left(0.67876\times10^{-6}\right)=-\left[\frac{6.73\left(0.67876\times10^{-6}\right)+4.3025\times10^{-7}}{2.316\times10^{-11}\left(0.67876\times10^{-6}\right)}\right]$$
$$=-3.1796\times10^{11}$$

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

$$|\in_t|=\left|\frac{190140-(190140)}{190140}\right|\times100\%$$
$$=0.00024868\ \%$$