Chemical Engineering Examples for the Romberg Rule for Integration

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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

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

Table 1 Values obtained using multiple-segment Trapezoidal rule.

n	Value
1	191190
2	190420
3	190260
4	190200

a) Use Romberg's rule to find the time required for 50 % of the oxygen to be consumed. Use the 2-segment and 4-segment Trapezoidal rule results given in Table 1.
b) Find the true error, E_t, for part (a).
c) Find the absolute relative true error, $|\in_t|$, for part (a).

Solution

a) $I_2=190420\text{ s}$

$I_4=190200\text{ s}$

Using Richardson's extrapolation formula for Trapezoidal rule

$$TV \approx I_{2n} + \frac{I_{2n} - I_n}{3}$$

and choosing n=2,

$$TV \approx I_4 + \frac{I_4 - I_2}{3}$$

$$= 190200 + \frac{190200 - (190420)}{3}$$

$$= 190130 \text{ s}$$

b) The exact value of the above integral is,

$$T = -\int_{1.22\times10^{-6}}^{0.61\times10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx$$

$$= 1.90140 \times 10^5 \text{ s}$$

so the true error is

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

$$= 1.9014 \times 10^5 - 190130$$

$$= 8.3322$$

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

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

$$= \left| \frac{8.3322}{1.90140 \times 10^5} \right| \times 100$$

$$= 0.0043823\,\%$$

Table 2 shows the Richardson's extrapolation results using 1, 2, 4, 8 segments. Results are compared with those of Trapezoidal rule.

Table 2 Values obtained using Richardson's extrapolation formula for Trapezoidal rule for

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

n	Trapezoidal Rule	$\lvert\in_t\rvert$ for Trapezoidal Rule %	Richardson's Extrapolation	$\lvert\in_t\rvert$ for Richardson's Extrapolation %
1	191190	0.55549	--	--
2	190420	0.14838	190163	0.014902
4	190210	0.037877	190127	0.0043823
8	190150	0.0095231	190133	0.00087599

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

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

Table 1 Values obtained using multiple-segment Trapezoidal rule.

n	Value
1	191190
2	190420
3	190260
4	190200
5	190180
6	190170
7	190160
8	190150

Use Romberg's rule to find the time required for 50 % of the oxygen to be consumed. Use the 1, 2, 4, and 8-segment Trapezoidal rule results as given in the Table 1.

Solution

From Table 1, the needed values from original Trapezoidal rule are

$$I_{1,1} = 191190 \text{ s}$$

$$I_{1,2} = 190420 \text{ s}$$

$$I_{1,3} = 190200 \text{ s}$$

$$I_{1,4} = 190150 \text{ s}$$

where the above four values correspond to using 1, 2, 4 and 8 segment Trapezoidal rule, respectively. To get the first order extrapolation values,

$$I_{2,1} = I_{1,2} + \frac{I_{1,2} - I_{1,1}}{3}$$

$$= 190420 + \frac{190420 - (191190)}{3}$$

$$= 190160 \text{ s}$$

Similarly

$$I_{2,2} = I_{1,3} + \frac{I_{1,3} - I_{1,2}}{3}$$

$$= 190200 + \frac{190200 - (190420)}{3}$$

$$= 190130 \text{ s}$$

$$I_{2,3} = I_{1,4} + \frac{I_{1,4} - I_{1,3}}{3}$$

$$= 190150 + \frac{190150 - (190200)}{3}$$

$$= 190130 \text{ s}$$

For the second order extrapolation values,

$$I_{3,1} = I_{2,2} + \frac{I_{2,2} - I_{2,1}}{15}$$

$$= 190130 + \frac{190130 - (190160)}{15}$$

$$= 190120 \text{ s}$$

Similarly

$$I_{3,2} = I_{2,3} + \frac{I_{2,3} - I_{2,2}}{15}$$

$$= 190130 + \frac{190130 - (190130)}{15}$$

$$= 190130 \text{ s}$$

For the third order extrapolation values,

$$I_{4,1} = I_{3,2} + \frac{I_{3,2} - I_{3,1}}{63}$$

$$= 190130 + \frac{190130 - (190120)}{63}$$

$$= 190130 \text{ s}$$

Table 2 shows these increased correct values in a tree graph.

Table 2 Improved estimates of value of integral using Romberg integration.

		1st Order	2nd Order	3rd Order
1-segment	191190			
		190160		
			190120	
2-segment	190420			
				190130
		190130		
			190130	
4-segment	190200			
		190130		
8-segment	190150			