Application of Numerical Integration in Solving a Reverse Osmosis Model

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Abstract. Clean water is always needed for human living. Due to pollution, we often need to purify water. One way to do so is using the reverse osmosis system. A mathematical model for the reverse osmosis system has been obtained. In this paper, we show the importance of numerical methods in solving the reverse osmosis model. In particular, we focus on the application of numerical integration methods in the process of solving the model. We consider three types of rules in numerical integration, namely, the Riemann sums, the trapezoidal rule and the Simpson's rule. We present our research results of these three rules relating to the solving process of our reverse osmosis model. The Simpson's rule is the most accurate, as it has the highest order of accuracy in comparison to the Riemann sums and the trapezoidal rule. Our main point in this research is that the numerical integration has an important role in solving the reverse osmosis model.

INTRODUCTION

Water is one source of life for living things on earth. However, some available water has now been heavily polluted by various types of waste and garbage from the results of human activities [1]. Therefore, a technique is needed to filter existing water. One of the water purification techniques is the reverse osmosis system. The reverse osmosis system is the process of separating and removing dissolved, organic, pyrogenic, colloidal submicrons, colors, nitrates, and bacteria from water using a semipermeable membrane [2]. In reverse osmosis the high pressure is given to the concentrated side of the membrane. When pressure is applied to this side, pure water will flow through the semipermeable membrane towards the other side of the lower concentration [3].

The process of distribution of concentration with space and time is described by parabolic type partial differential equations known as advection-diffusion equations. The advection-diffusion equation is a model that can be used to simulate the spread of pollutants [4]. This mathematical model for the reverse osmosis system has been obtained [5].

In this paper, we show the importance of numerical integration in solving the reverse osmosis mathematical model. Numerical integration has many applications in the field of applied mathematics, especially in mathematical physics and computational chemistry [6]. Numerical integration is a technique for calculating integrals which are difficult to solve analytically. We compare three types of rules in numerical integration, the Riemann sums, the trapezoidal rule, and Simpson's rules. Three types of Riemann sums are the left Riemann sum, the right Riemann sum, and the middle Riemann sum. Some authors (see [7, 8, 9]) have applied some of the three numerical integration rules to find solutions to a mathematical model. General formula for the Riemann sum rule is given in [10]:

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} f(x_i^*)\Delta x. \tag{1}$$

International Conference on Science and Applied Science (ICSAS) 2019
AIP Conf. Proc. 2202, 020043-1–020043-6; https://doi.org/10.1063/1.5141656
Published by AIP Publishing. 978-0-7354-1953-7/$30.00

with $x_i^* = x_i$ for the right Riemann sum, $x_i^* = x_{i-1}$ for the left Riemann sum, and $x_i^* = (x_i + x_{i-1})/2$ for the middle Riemann sum. The general formula for the trapezoidal rule is given by [10]:

$$\int_a^b f(x)dx \quad \approx \frac{h}{2}\left(f_0 + 2\sum_{i=1}^{n-1} f_i + f_n\right) \tag{2}$$

where $f_i = f(x_i)$, $x_0 = a$, and $x_n = b$. The general formula for the Simpson's rule is given by [10]:

$$\int_a^b f(x)dx \quad \approx \frac{h}{3}\left(f_0 + 4\sum_{i=1}^{M} f_{2i-1} + 2\sum_{i=1}^{M-1} f_{2i} + f_{2M}\right) \tag{3}$$

where $n = 2M$ and M is a positive integer. In this paper, we also calculate errors from the five rules of numerical integration.

The rest of this paper consists of the mathematical model, application of numerical integration, discussion of results, and conclusions.

MATHEMATICAL MODEL

The mathematical model for predicting the concentration of salt solutions in semipermeable membranes in the reverse osmosis system is as follows [5]:

$$y\frac{\partial C}{\partial x} = \alpha\frac{\partial^2 C}{\partial y^2}, \tag{4}$$

with $\alpha = \frac{Dh}{v_0}$ and the boundary conditions are

$$C(0, y) = c_0, \;\; C(x, \infty) = c_0 \tag{5}$$

and

$$-D\frac{\partial C}{\partial y}(x, 0) = qC(x, 0) \tag{6}$$

where x and y are space variables. $C = C(x, y)$ represents the concentration of salt solution in a semipermeable membrane at point (x, y). Notations q, D, h, c_0, and v_0 are, respectively, water flow rates in semipermeable distribution, salt diffusivity in water, distance from the semipermeable boundary to the center of the channel, concentration away from semipermeable membranes, and horizontal velocity measured at a distance h from the semipermeable boundary. Here q, D, h, and v_0 are constants.

APPLICATION OF NUMERICAL INTEGRATION

The solutions of equations (4), (5), and (6) are as follows [5]:

$$C(x, 0) = \quad \frac{3^{-\frac{1}{3}}qc_0}{DI}\left(\frac{Dh}{v_0}\right)^{1/3} x^{\frac{1}{3}} + c_0, \tag{7}$$

with $I = \int_0^\infty e^{-v^3} v\, dv.$ Equation (7) is an equation that is used to predict the concentration of salt solutions in semipermeable membranes in the reverse osmosis system.

In equation (7) there is a definite integral I which is very difficult to solve analytically. Therefore, we solve the definite integral I using the left Riemann sum rule, right Riemann sum rule, and middle Riemann sum rule, trapezoidal rule, and Simpson's rule.

In all calculations the same interval is used, namely [0, 10]. This interval [0, 10] is partitioned into $n = 200$ subintervals namely $[v_0, v_1]$, $[v_1, v_2]$, $[v_2, v_3]$, … , $[v_{199}, v_{200}]$ with $v_0 = 0$ and $v_n = 10$ where $\Delta v = \frac{10-0}{200} = 0.05$ is uniform, as shown in Fig. 1.

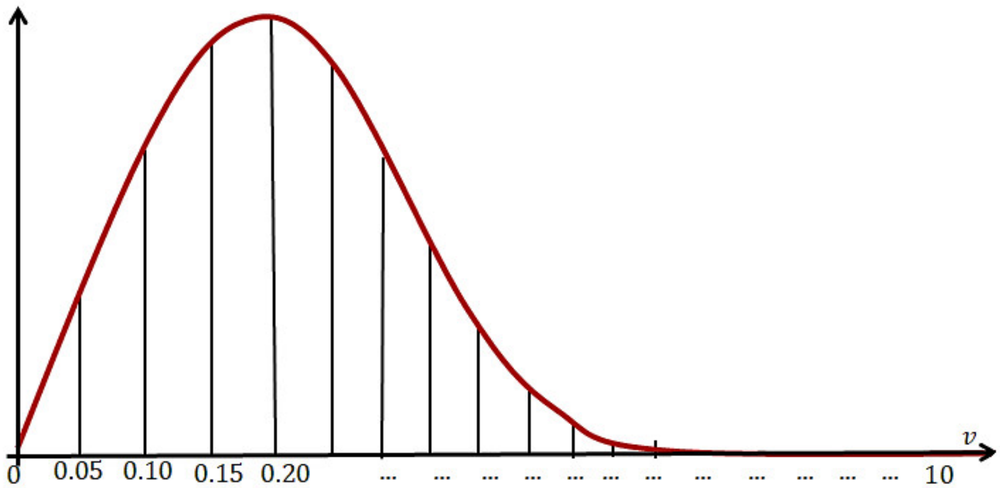

FIGURE 1. Graph of function $f(v)$

Right Riemann Sum

Based on the right Riemann sum formula, $v_i = 0.05$ is chosen as the right end point of the interval $[0,10]$ with $i = 0.05,\ 0.10,\ 0.15, \dots,\ 200$, so that we obtain

$$\begin{aligned}
\int_0^{10} e^{-v^3} v\, dv \quad &\approx \sum_{i=0.05}^{2000} (\, e^{-{v_i}^3} v_i)(0.05) \\
&\approx f(x_0^*)\Delta v + f(x_1^*)\Delta v + \cdots + f(x_n^*)\Delta v \\
&\approx f(0.05)(0.05) + f(0.10)(0.05) + \cdots + f(10)(0.05) \\
&\approx \left(e^{-0.05^3} 0.05\right)(0.05) + \left(e^{-0.10^3} 0.10\right)(0.05) + \cdots + (e^{-100^3} 10)(0.05) \\
&\approx (0.04999375)(0.05) + (0.09990005)(0.05) + \cdots + (0)(0.05) \\
&\approx (0.002499688) + (0.004995002) + \cdots + (0)
\end{aligned}$$

$$\int_0^{10} e^{-v^3} v\, dv \approx 0.4511643131.$$

Thus, the approximation of the I value is obtained using the right Riemann sum rule, which is 0.4511643131.

Left Riemann Sum

Based on the right Riemann sum formula, $v_i = 0.05$ is chosen as the right end point of the interval from each subinterval $[0,10]$ with $i = 0.05, 0.10, 0.15, \dots, 200$, so that we obtain

$$\begin{aligned}
\int_0^{10} e^{-v^3} v\, dv \quad &\approx \sum_{i=0}^{199} (e^{-{v_i}^3} v_i)(0.05) \\
&\approx f(v_0^*)\Delta v + f(v_1^*)\Delta v + \cdots + f(v_{n-1}^*)\Delta v \\
&\approx f(0)(0) + f(0.05)(0.05) + \cdots + f(9.95)(0.05) \\
&\approx \left(e^{-0^3}.\, 0\right)(0.05) + \left(e^{-0.05^3} 0.05\right)(0.05) + \cdots + (e^{-9.95^3} 9.95)(0.05) \\
&\approx (0)(0.05) + (0.04999375)(0.05) + \cdots + (0)(0.05) \\
&\approx (0) + (0.002499688) + (0.004995002) + \cdots + (0)
\end{aligned}$$

$$\int_0^{10} e^{-v^3} v\, dv \approx\ 0.4511643131.$$

Thus, the approximation of the I value is obtained using the left Riemann sum rule, which is 0.4511643131.

Middle Riemann Sum

In the middle Riemann sum rule, $\bar{v}_i$ is chosen as the midpoint of each subinterval at $[0{,}10]$ with $i = 0, 1, 2, \ldots, 200$, so that based on the middle Riemann sum we obtain

$$\int_0^{10} e^{-v^3} v \, dv \approx \sum_{i=0}^{200} f(\bar{v}_i) \Delta v$$

with $\Delta v = 0.05$ and $\bar{v}_i = \frac{1}{2}(v_{i-1} + v_i)$, as listed in Table 1.

TABLE 1. Value of $\bar{v}_i$ for summation of middle Riemann

v_{i-1}	v_i	$\bar{v}_i$
0	0.05	0.025
0.05	0.10	0.075
0.10	0.15	0.125
…	…	…
9.95	10	9.975

Furthermore, the value of $\bar{v}_i$ in Table 1 is substituted to the middle Riemann sum formula as follows

$$\begin{aligned}
\int_0^{10} e^{-v^3} v \, dv &\approx \sum_{i=0}^{200} (e^{-v_i{}^3} v_i)(0.05) \\
&\approx f(v_0^*)\Delta v + f(v_1^*)\Delta v + f(v_2^*)\Delta v + \cdots + f(v_{n-1}^*)\Delta v \\
&\approx f(0.025)(0) + f(0.075)(0.05) + \cdots + f(9.975)(0.05) \\
&\approx \left(e^{-0.025^3} 0.025\right)(0.05) + \left(e^{-0.075^3} 0.075\right)(0.05) + \cdots + (e^{-9.975^3} 9.975)(0.05) \\
&\approx (0.024999609)(0.05) + (0.074968366)(0.05) + \cdots + (0)(0.05) \\
&\approx (0.00124998) + (0.003748418) + \cdots + (0) \\
&\approx 0.451476813.
\end{aligned}$$

Thus, the approximation of the I value is obtained using the middle Riemann sum rule, which is 0.451476813.

Trapezoidal Rule

Based on the trapezoidal rule formula, at interval $[0{,}10]$ which is divided into 200 intervals the section $[v_0, v_{200}]$ as wide as $\Delta v = 0.05$ by using a partition point that is equidistant, that is, $v_i = 0 + i\Delta v$, $i = 0, 1, 2, \ldots, 200$, we obtain

$$\begin{aligned}
\int_0^{10} e^{-v^3} v \, dv &\approx \frac{\Delta v}{2}\left(f(v_0) + 2\sum_{i=1}^{n-1} f(v_i) + f(v_{200}) \right) \\
&\approx \frac{0.05}{2}\left(f(0) + 2f(0.05) + 2f(0.10) + \cdots + f(10)\right) \\
&\approx \frac{0.05}{2}\left(\left(e^{-0^3} 0\right) + 2e^{-0.05^3} 0.05 + \cdots + \left(e^{-10^3} 10\right)\right) \\
&\approx \frac{0.05}{2}\left((0) + 2(0.04999375) + \cdots + (0)\right) \\
&\approx 0.4511643131.
\end{aligned}$$

Thus, the approximation of the I value is obtained by using the trapezoidal rule of 0.4511643131.

Simpson's Rule

Based on the Simpson's rule formula $1/3$, for the interval $[0{,}10]$ is divided into $2M = 200$ intervals, the section $[v_0, v_{200}]$ is equal to that of $\Delta v = 0.05$ and uses partition points that are equidistant, that is, $v_i = 0 + ih$, $i = 0, 1, 2, \ldots, 2M$, then

$$
\begin{aligned}
\int_0^{10} e^{-v^3} v\,dv &\approx \frac{\Delta v}{3}\left(f_0 + 4\sum_{i=1}^{M} f_{2i-1} + 2\sum_{i=1}^{M-1} f_{2i} + f_{200}\right) \\
&\approx \frac{0.05}{3}\left(f_0 + 4\sum_{i=1}^{100} f_{2i-1} + 2\sum_{i=1}^{99} f_{2i} + f_{200}\right) \\
&\approx \frac{0.05}{3}(f_0 + 4f_1 + 2f_2 + \cdots + 4f_{199} + f_{200}) \\
&\approx \frac{0.05}{3}(e^{-0^3}0 + 4e^{-0.05^3}0.05 + \cdots + 4e^{-9.95^3}9.95 + e^{-10^3}10) \\
&\approx (0.016666667)(27.08235879) \\
\int_0^{10} e^{-v^3} v\,dv &\approx 0.4513726464.
\end{aligned}
$$

Thus, the approximation of the I value is obtained using the Simpson $1/3$ rule, which is 0.4513726464.

DISCUSSION

In this section, we discuss the accuracy of calculating the five rules of numerical integration above. The exact value of I is obtained using the Maple program, as follows:

$$I = \int_0^{\infty} e^{-v^3} v\,dv = 0.4513726463.$$

Based on the results of the calculation of the definite integral I in section 3, the error of the left Riemann sum rule, the right Riemann sum rule, the middle Riemann sum rule, the trapezoidal rule, and the Simpson's rule are given in Table 2.

TABLE 2. Results of each numerical integration rule

Integration Rule	Exact of Maple	Numerical results	Error
Left Riemann sum rule	0.4513726463	0.4511643131	0.0002083332
Right Riemann sum rule	0.4513726463	0.4511643131	0.0002083332
Middle Riemann sum rule	0.4513726463	0.4514768131	0.0001041668
Trapezoidal rule	0.4513726463	0.4511643131	0.0002083332
Simpson's rule	0.4513726463	0.4513726464	0.0000000001

Based on the error calculation in Table 2, the error of the Simpson's rule is smaller than those of the other four numerical integration rules. This is because the Simpson's rule has a higher order of accuracy than the other four numerical integration rules. Thus, we use the value I of the Simpson's rule as the most accurate I value. This value of I is substituted to equation (7), so that we obtain

$$\frac{C(x,0)}{c_0} = 1.5361171751\left(\frac{q}{D}\right)\left(\frac{Dh}{v_0}\right)^{1/3} x^{\frac{1}{3}} + 1\,. \tag{8}$$

Equation (8) is a mathematical equation to predict the concentration of salt solutions in semipermeable membranes in the reverse osmosis system.

CONCLUSION

Numerical integration has an important role in solving the reverse osmosis model. The more accurate the the integral value that we obtain, the more accurate results of the mathematical model we will get. Based on the calculation of the numerical integration, the Simpson's rule is the most accurate rule compared to the left Riemann sum rule, right Riemann sum rule, middle Riemann sum rule, and trapezoidal rule.