



Multi-Step DTM simulation of Transesterification reactions model

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Abstract

The multi-step differential transform method (DTM) adopted from the standard DTM is employed in this case study to solve a model of the transesterification reaction. The DTM is considered in a sequence of time intervals. The accuracy of the proposed method is confirmed by comparing its results with those of the fourth-order RungeKutta (RK4) method. In addition, the experimental results are investigated with the Multi-step DTM to demonstrate the efficiency and effectiveness of these chemical reactions obtained in the laboratory. The present findings confirmed the effectiveness of using the multi-step DTM in validating the chemical models obtained in laboratories.

Keywords. Multi-step DTM, transesterification reaction, RK4 method, Numerical solution.

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1. INTRODUCTION

Increasing attention has been paid to renewable energy sources to compensate for the diminishing fossil fuels, growing oil prices, and the environmental pollution caused by consuming fossil fuels [1, 2]. As a renewable energy source, biodiesel production is produced through the transesterification of triglyceride as the main component of animal fats and vegetable oils or through the esterification of free fatty acids with short-chain alcohol, mainly including methanol [3, 4]. Biodiesel is biodegradable, renewable, environmentally friendly, and non-toxic and these results illustrated that biodiesel can be utilized in compression-ignition (diesel) engines with little or without modification due to its adjustable chemical and physical properties [5–7]. Biodiesel has producing much less sulfur dioxide, carbon monoxide, and unburned hydrocarbons compared to petroleum-based diesel fuel so it has favorable combustion emission profile [8, 9]. During the chemical process of transesterification, biodiesel is generated as a result of a reaction between triglycerides and methanol or ethanol, which yields ethyl or methyl esters of fatty acids and glycerol [10]. Today, commercial biodiesel is produced in transesterification reactions in which acid or alkaline catalysts are employed [11]. Transesterification can involve equilibrium reactions in supercritical methanol conditions. This study adopted the consecutive transesterification reaction as a three-step thoroughly-reversible model. Empirical evidence suggests diolein can be generated through an irreversible reaction between triolein and methanol. Monoolein is also generated through a reversible reaction between diolein and methanol. Glycerol is ultimately produced through a reversible

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reaction between monoolein and methanol. The following equation shows these reactions:



accordingly, the kinetics of the transesterification process is expressed as [12]:

$$\begin{aligned} \frac{dX_{TO}}{dt} &= -\frac{1}{M_{wMeOH}} k_1 X_{TO} X_{MeOH}, \\ \frac{dX_{DO}}{dt} &= \frac{M_{wDO}}{M_{wTO} \times M_{wMeOH}} k_1 X_{TO} X_{MeOH} - \frac{1}{M_{wMeOH}} k_2 X_{DO} X_{MeOH} \\ &\quad + \frac{M_{wDO}}{M_{wMO} \times M_{wME}} k_{-2} X_{MO} X_{ME}, \\ \frac{dX_{MO}}{dt} &= \frac{M_{wMO}}{M_{wDO} \times M_{wMeOH}} k_2 X_{DO} X_{MeOH} - \frac{1}{M_{wME}} k_{-2} X_{MO} X_{ME} \\ &\quad - \frac{1}{M_{wMeOH}} k_3 X_{MO} X_{MeOH} + \frac{M_{wMO}}{M_{wGL} \times M_{wME}} k_{-3} X_{GL} X_{ME}, \\ \frac{dX_{MeOH}}{dt} &= -\frac{1}{M_{wTO}} k_1 X_{TO} X_{MeOH} - \frac{1}{M_{wDO}} k_2 X_{DO} X_{MeOH} - \frac{1}{M_{wMO}} k_3 X_{MO} X_{MeOH} \\ &\quad + \frac{M_{wMeOH}}{M_{wMO} \times M_{wME}} k_{-2} X_{MO} X_{ME} + \frac{M_{wMeOH}}{M_{wGL} \times M_{wME}} k_{-3} X_{GL} X_{ME}, \\ \frac{dX_{ME}}{dt} &= \frac{M_{wME}}{M_{wTO} \times M_{wMeOH}} k_1 X_{TO} X_{MeOH} + \frac{M_{wME}}{M_{wDO} \times M_{wMeOH}} k_2 X_{DO} X_{MeOH} \\ &\quad + \frac{M_{wME}}{M_{wMO} \times M_{wMeOH}} k_3 X_{MO} X_{MeOH} - \frac{1}{M_{wMO}} k_{-2} X_{MO} X_{ME} - \frac{1}{M_{wGL}} k_{-3} X_{GL} X_{ME}, \\ \frac{dX_{GL}}{dt} &= \frac{M_{wGL}}{M_{wMO} \times M_{wMeOH}} k_3 X_{MO} X_{MeOH} - \frac{1}{M_{wME}} k_{-3} X_{GL} X_{ME}. \end{aligned} \quad (1.4)$$

with initial condition:

$$X_{TO}(0) = 75, \quad X_{DO}(0) = 0, \quad X_{MO}(0) = 0, \quad X_{MeOH}(0) = 23, \quad X_{ME}(0) = 0, \quad X_{GL}(0) = 0, \quad (1.5)$$

where Mw is defined as the molecular weight of components (for TO, DO, ME, MO, GL, and methanol (MeOH) are 885, 621, 356, 296.5, 92, and 32 g/mol respectively). X and t are the component's content (wt%) and reaction time (min). The present study employed the DTM to estimate an analytical solution to the system (1.4) with initial

TABLE 1. Constants for the proposed mechanism, wt% the unit.

k	k_1	k_2	k_{-2}	k_3	k_{-3}
$g.mol^{-1}min^{-1}$	2.88	4.40	1.06	12.75	1.95

condition (1.5) in a sequence of time intervals. The proposed technique was referred to as the multi-step DTM. The DTM introduced by Zhou [13] was developed by other researchers [14–20]. Despite the shortcomings of the DTM, its application to a wide range of linear and nonlinear models has yielded promising outcomes in different scientific fields. The truncated series solution obtained in this study using the DTM did not present the actual behavior of the problem; rather, it provided a good enough estimate of the exact solution in a very limited area. The multi-step DTM was therefore developed [21] to improve the method's accuracy and the convergence rate of the series solution



to ordinary differential equations over a broader area. Applications of this multi-step technique to diverse physics and engineering problems have been well addressed in literature [22–28]. Also for more related papers, we refer the reader to [29–45]. This article was organized as follows in the remaining sections: Section 2 provides an overview of the DTM and its multi-step version. Section 3 applies the method to the model (1.4) with initial conditions (1.5). Section 4 performs a graphical numerical simulation by comparing the results of the multi-step method with those of the RK4 method and empirical data. This article is concluded in section 5.

2. MULTI-STEP DTM

Consider a nonlinear system of differential equations:

$$\begin{cases} \dot{w}_1(t) = g_1(t, w_1(t), w_2(t), \dots, w_n(t)), \\ \dot{w}_2(t) = g_2(t, w_1(t), w_2(t), \dots, w_n(t)), \\ \vdots \\ \dot{w}_n(t) = g_n(t, w_1(t), w_2(t), \dots, w_n(t)), \end{cases} \tag{2.1}$$

with initial conditions:

$$w_{i0}(t_0) = c_i, \quad i = 1, 2, \dots, n. \tag{2.2}$$

A solution to the initial-value problem (2.1)-(2.2) is obtained on the interval of $[t_0, L]$. The following finite series can be used in real-world applications of the DTM to estimate the solution to the initial value problem (2.1)-(2.2) as:

$$\begin{cases} w_1(t) \approx \sum_{l=0}^N W_1(l)(t - t_0)^l, \\ w_2(t) \approx \sum_{l=0}^N W_2(l)(t - t_0)^l, \\ \vdots \\ w_n(t) \approx \sum_{l=0}^N W_n(l)(t - t_0)^l, \end{cases} \tag{2.3}$$

where $W_i(l)$ is the differential transform for $w_i(t)$ and satisfies recurrence relation:

$$W_i(l + 1) = \frac{1}{l + 1} G_i(l, W_1(l), W_2(l), \dots, W_n(l)), \quad i = 1, 2, \dots, n. \tag{2.4}$$

$W_i(0) = c_i$ and $G_i(l, W_1(l), W_2(l), \dots, W_n(l))$ is the differential transform of function $g_i(t, w_1(t), \dots, w_n(t))$ for $i = 1, 2, \dots, n$. The estimated solution (2.3) is found invalid at large values of t . The initial estimate is therefore modified through a sequence of sub-intervals with an initial approximation to ensure the solution validity at a large t . Let $[t_0, L]$ be categorized into M subintervals of $[t_{m-1}, t_m]$, $m = 1, \dots, M$ of the same step size $h = \frac{L-t_0}{M}$ by employing $t_m = mh + t_0$ as nodes. The principal idea behind the multi-step DTM is expressed as follows: The initial condition $w_i(t_0) = c_i, i = 1, \dots, n$ is used to apply the DTM to equation (2.1) on $[t_0, t_1]$ and thus acquire an estimated solution $w_{i,1}, t \in [t_0, t_1]$. The initial condition, $w_{i,m}(t_{m-1}), m \geq 2$ is used on the subinterval $[t_{m-1}, t_m]$ to apply the DTM to equation (2.1) over $[t_{m-1}, t_m]$. This process is repeated to generate a sequence of estimated solutions. $w_{i,m}(t), m = 1, \dots, M, i = 1, \dots, n$. The following solution is ultimately obtained by utilizing the multi-step DTM:

$$w_i(t) = \begin{cases} w_{i,1}(t) & t \in [t_0, t_1], \\ w_{i,2}(t) & t \in [t_1, t_2], \\ \vdots \\ w_{i,M}(t) & t \in [t_{M-1}, t_M]. \end{cases} \tag{2.5}$$



3. NUMERICAL SIMULATION

This section applied the multi-step DTM to the transesterification reactions model.

By substituting:

$$x_1 = X_{TO}, \quad x_2 = X_{DO}, \quad x_3 = X_{MO}, \quad x_4 = X_{MeOH}, \quad x_5 = X_{ME}, \quad x_6 = X_{GL}. \quad (3.1)$$

in Eqs. (1.4) and (1.5), we have:

$$\begin{aligned} \dot{x}_1 &= -0.09x_1x_4, \\ \dot{x}_2 &= -0.0631x_1x_4 - 0.1375x_2x_4 + 0.0062x_3x_5, \\ \dot{x}_3 &= 0.0656x_2x_4 - 0.003x_3x_5 - 0.398x_3x_4 + 0.0143x_5x_6, \\ \dot{x}_4 &= -0.0034x_1x_4 - 0.0071x_2x_4 - 0.043x_3x_4 + 0.0003x_3x_5 + 0.0016x_5x_6, \\ \dot{x}_5 &= 0.0362x_1x_4 + 0.0789x_2x_4 + 0.478x_3x_4 - 0.0036x_3x_5 - 0.0173x_5x_6, \\ \dot{x}_6 &= 0.1236x_3x_4 - 0.0045x_5x_6. \end{aligned} \quad (3.2)$$

where initial condition:

$$x_1(0) = 75, \quad x_2(0) = 0, \quad x_3(0) = 0, \quad x_4(0) = 23, \quad x_5(0) = 0, \quad x_6(0) = 0. \quad (3.3)$$

By applying DTM to a nonlinear system of differential equations (3.2) with initial condition (3.3), the solution of the equations (3.2) is given by:

$$\begin{aligned} (l+1)X_1(l+1) &= -0.09 \sum_{\lambda=0}^l X_1(\lambda)X_4(l-\lambda), \\ (l+1)X_2(l+1) &= 0.0631 \sum_{\lambda=0}^l X_1(\lambda)X_4(l-\lambda) - 0.1375 \sum_{\lambda=0}^l X_2(\lambda)X_4(l-\lambda) + 0.0062 \sum_{\lambda=0}^l X_3(\lambda)X_5(l-\lambda), \\ (l+1)X_3(l+1) &= 0.0656 \sum_{\lambda=0}^l X_2(\lambda)X_4(l-\lambda) - 0.003 \sum_{\lambda=0}^l X_3(\lambda)X_5(l-\lambda) \\ &\quad - 0.398 \sum_{\lambda=0}^l X_3(\lambda)X_4(l-\lambda) + 0.0143 \sum_{\lambda=0}^l X_5(\lambda)X_6(l-\lambda) \\ (l+1)X_4(l+1) &= -0.0034 \sum_{\lambda=0}^l X_1(\lambda)X_4(l-\lambda) - 0.0071 \sum_{\lambda=0}^l X_2(\lambda)X_4(l-\lambda) \\ &\quad - 0.043 \sum_{\lambda=0}^l X_3(\lambda)X_4(l-\lambda) + 0.0016 \sum_{\lambda=0}^l X_3(\lambda)X_5(l-\lambda), \\ (l+1)X_5(l+1) &= 0.0362 \sum_{\lambda=0}^l X_1(\lambda)X_4(l-\lambda) + 0.0789 \sum_{\lambda=0}^l X_2(\lambda)X_4(l-\lambda) \\ &\quad + 0.478 \sum_{\lambda=0}^l X_3(\lambda)X_4(l-\lambda) - 0.0036 \sum_{\lambda=0}^l X_3(\lambda)X_5(l-\lambda) \\ &\quad - 0.0173 \sum_{\lambda=0}^l X_5(\lambda)X_6(l-\lambda), \end{aligned} \quad (3.4)$$



$$(l + 1)X_6(l + 1) = 0.1236 \sum_{\lambda=0}^l X_3(\lambda)X_4(l - \lambda) - 0.0045 \sum_{\lambda=0}^l X_5(\lambda)X_6(l - \lambda).$$

with initial condition:

$$X_1(0) = 75, \quad X_2(0) = 0, \quad X_3(0) = 0, \quad X_4(0) = 23, \quad X_5(0) = 0, \quad X_6(0) = 0. \tag{3.5}$$

Therefore, according to DTM the n -term approximations for a linear system of differential equations (3.2) can be expressed as:

$$\begin{aligned} x_1 &= \sum_{l=0}^n X_1(l)t^l, \\ x_2 &= \sum_{l=0}^n X_2(l)t^l, \\ x_3 &= \sum_{l=0}^n X_3(l)t^l, \\ x_4 &= \sum_{l=0}^n X_4(l)t^l, \\ x_5 &= \sum_{l=0}^n X_5(l)t^l, \\ x_6 &= \sum_{l=0}^n X_6(l)t^l. \end{aligned} \tag{3.6}$$

In addition, $X_{1,i}(t), X_{2,i}(t), \dots, X_{6,i}(t)$ which satisfies the following recurrence equations for $i = 1, \dots, M$ are obtained by applying the multi-step method to a linear differential equation system (3.2) with initial conditions (2.3) as:

$$\begin{aligned} (l + 1)X_{1,i}(l + 1) &= -0.09 \sum_{\lambda=0}^l X_{1,i}(\lambda)X_{4,i}(l - \lambda), \\ (l + 1)X_{2,i}(l + 1) &= 0.0631 \sum_{\lambda=0}^l X_{1,i}(\lambda)X_{4,i}(l - \lambda) - 0.1375 \sum_{\lambda=0}^l X_{2,i}(\lambda)X_{4,i}(l - \lambda) \\ &\quad + 0.0062 \sum_{\lambda=0}^l X_{3,i}(\lambda)X_{5,i}(l - \lambda), \\ (l + 1)X_{3,i}(l + 1) &= 0.0656 \sum_{\lambda=0}^l X_{2,i}(\lambda)X_{4,i}(l - \lambda) - 0.003 \sum_{\lambda=0}^l X_{3,i}(\lambda)X_{5,i}(l - \lambda) \\ &\quad - 0.398 \sum_{\lambda=0}^l X_{3,i}(\lambda)X_{4,i}(l - \lambda) + 0.0143 \sum_{\lambda=0}^l X_{5,i}(\lambda)X_{6,i}(l - \lambda), \\ (l + 1)X_{4,i}(l + 1) &= -0.0034 \sum_{\lambda=0}^l X_{1,i}(\lambda)X_{4,i}(l - \lambda) - 0.0071 \sum_{\lambda=0}^l X_{2,i}(\lambda)X_{4,i}(l - \lambda) \\ &\quad - 0.043 \sum_{\lambda=0}^l X_{3,i}(\lambda)X_{4,i}(l - \lambda) + 0.0016 \sum_{\lambda=0}^l X_{3,i}(\lambda)X_{5,i}(l - \lambda), \end{aligned} \tag{3.7}$$



$$\begin{aligned}
(l+1)X_{5,i}(l+1) &= 0.0362 \sum_{\lambda=0}^l X_{1,i}(\lambda)X_{4,i}(l-\lambda) + 0.0789 \sum_{\lambda=0}^l X_{2,i}(\lambda)X_{4,i}(l-\lambda) + 0.478 \sum_{\lambda=0}^l X_{3,i}(\lambda)X_{4,i}(l-\lambda) \\
&\quad - 0.0036 \sum_{\lambda=0}^l X_{3,i}(\lambda)X_{5,i}(l-\lambda) - 0.0173 \sum_{\lambda=0}^l X_{5,i}(\lambda)X_{6,i}(l-\lambda), \\
(l+1)X_{6,i}(l+1) &= 0.1236 \sum_{\lambda=0}^l X_{3,i}(\lambda)X_{4,i}(l-\lambda) - 0.0045 \sum_{\lambda=0}^l X_{5,i}(\lambda)X_{6,i}(l-\lambda).
\end{aligned}$$

with initial condition:

$$\begin{aligned}
X_{1,i}(0) &= 75, \quad X_{2,i}(0) = 0, \quad X_{3,i}(0) = 0, \quad X_{4,i}(0) = 23, \quad X_{5,i}(0) = 0, \quad X_{6,i}(0) = 0, \\
X_{1,i}(0) &= X_{1,i-1}(t_i), \quad X_{2,i}(0) = X_{1,i-1}(t_i), \quad X_{3,i}(0) = X_{1,i-1}(t_i), \\
X_{4,i}(0) &= X_{1,i-1}(t_i), \quad X_{5,i}(0) = X_{1,i-1}(t_i), \quad X_{6,i}(0) = X_{1,i-1}(t_i).
\end{aligned} \tag{3.8}$$

For $i = 1, 2, \dots, M$.

According to multi-step DTM, the series solution for the system is suggested by:

$$\begin{aligned}
x_1 &= \begin{cases} \sum_{l=0}^n X_{1,1}(l)t^l & t \in [0, t_1], \\ \sum_{l=0}^n X_{1,2}(l)(t-t_1)^l & t \in [t_1, t_2], \\ \vdots \\ \sum_{l=0}^n X_{1,M}(l)(t-t_{M-1})^l & t \in [t_{M-1}, t_M], \end{cases} \\
x_2 &= \begin{cases} \sum_{l=0}^n X_{2,1}(l)t^l & t \in [0, t_1], \\ \sum_{l=0}^n X_{2,2}(l)(t-t_1)^l & t \in [t_1, t_2], \\ \vdots \\ \sum_{l=0}^n X_{2,M}(l)(t-t_{M-1})^l & t \in [t_{M-1}, t_M], \end{cases} \\
&\vdots \\
x_6 &= \begin{cases} \sum_{l=0}^n X_{6,1}(l)t^l & t \in [0, t_1], \\ \sum_{l=0}^n X_{6,2}(l)(t-t_1)^l & t \in [t_1, t_2], \\ \vdots \\ \sum_{l=0}^n X_{6,M}(l)(t-t_{M-1})^l & t \in [t_{M-1}, t_M]. \end{cases}
\end{aligned} \tag{3.9}$$



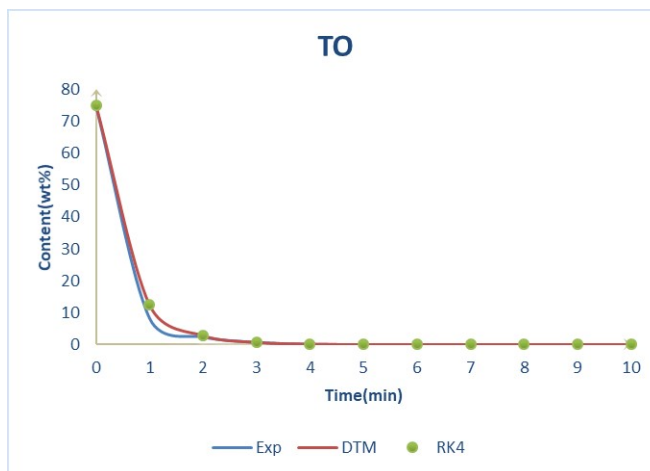


FIGURE 1. Multi-step DTM and RK4 numerical comparisons with experimental results of X_{TO} .

4. RESULTS AND DISCUSSION

For the following cases, the tenth term of the solution obtained from the Multi-step DTM with a step size of 0.01 is compared with that of the RK4 method with a step size of $\Delta t = 0.001$. The numerical data obtained from the multi-step technique, the RK4 method, and experimental results as well as the empirical findings are presented in Figures 1-5 and Tables 2-5. Results showed that, there is a good harmony between the experimental and predicted values.

TABLE 2. Multi-step DTM and RK4 numerical comparisons with experimental results of X_{TO} .

t	$X_{TO,DTM}$	$X_{TO,RK4}$	$X_{TO,exp.}$
0	75	75	75
1	12.48238	12.48468	8.3665
2	2.86572	2.869497	2.4586
3	0.719085	0.720702	0.7645
4	0.184381	0.184963	0.1152
5	0.047453	0.047647	0.0735
6	0.0122	0.012261	0.0521
7	0.003129	0.003147	0.0476
8	0.0008	0.000806	0.0432
9	0.000204	0.000205	0.0323
10	0.00051	0.00052	0.0303

5. CONCLUSION

In this study, we have used multi-step DTM to obtain a numerical solution for the transesterification reaction model. The obtained findings were compared with empirical data and those obtained from the RK4 method, which



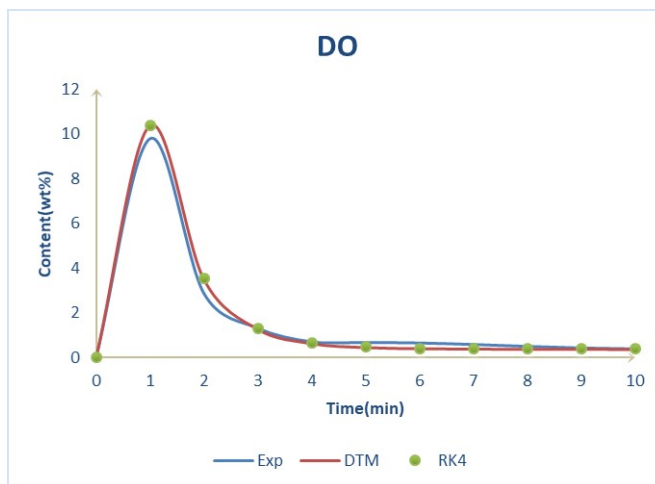


FIGURE 2. Multi-step DTM and RK4 numerical comparisons with experimental results of X_{DO} .

TABLE 3. Multi-step DTM and RK4 numerical comparisons with experimental results of X_{DO} .

t	$X_{DO,DTM}$	$X_{DO,RK4}$	$X_{DO,exp.}$
0	0	0	0
1	10.39083	10.39805	9.7898
2	3.51547	3.513418	2.8865
3	1.277603	1.276013	1.3315
4	0.635728	0.635049	0.7186
5	0.457761	0.45752	0.6889
6	0.407457	0.407379	0.6656
7	0.391284	0.391261	0.5986
8	0.384111	0.384105	0.5138
9	0.379316	0.379315	0.4426
10	0.375175	0.375176	0.4022

was utilized as a benchmark for the comparisons. Due to the reduced computational burden and high accuracy achieved by using multi-step DTM, this technique plays a key role in solving a wide range of chemical problems. This method was directly employed without applying discretization, linearization, and perturbation. All the calculations were also performed in Maple13. The results indicated that the multi-step DTM new algorithm increased the interval of convergence for the series solution. Obviously, the accuracy can be improved when the step size h and the number of terms in each subinterval K become smaller and larger respectively. This manuscript was shown that the proposed algorithm is a very accurate and efficient method compared with the RK4 method for both non-chaotic and chaotic systems. The method worked successfully in handling systems of differential equations directly with a minimum size of computations and a wide interval of convergence for the series solution. This emphasizes the fact that the Multi-step DTM applies to many other nonlinear models and its reliable and promising when compared with existing methods.



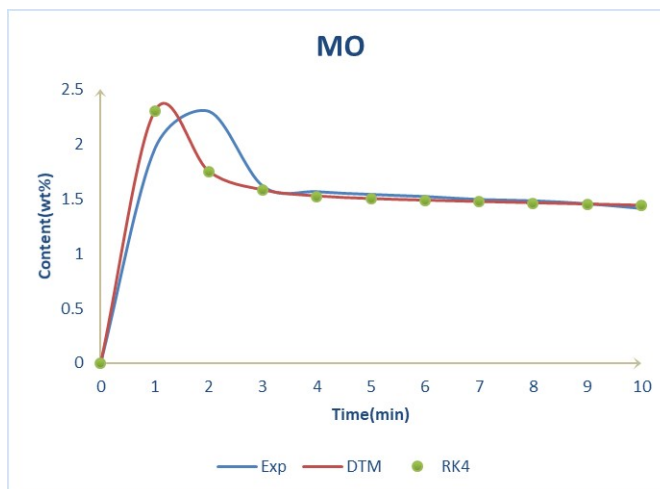


FIGURE 3. Multi-step DTM and RK4 numerical comparisons with experimental results of X_{MO} .

TABLE 4. Multi-step DTM and RK4 numerical comparisons with experimental results of X_{MO} .

t	$X_{MO,DTM}$	$X_{MO,RK4}$	$X_{MO,exp.}$
0	0	0	0
1	2.298527	2.299983	1.9611
2	1.746371	1.746331	2.3025
3	1.577992	1.577905	1.6164
4	1.522953	1.522914	1.5666
5	1.499349	1.499338	1.5415
6	1.484616	1.484615	1.5223
7	1.472394	1.472397	1.49542
8	1.460928	1.460933	1.4832
9	1.449745	1.44975	1.4565
10	1.438718	1.438723	1.4135

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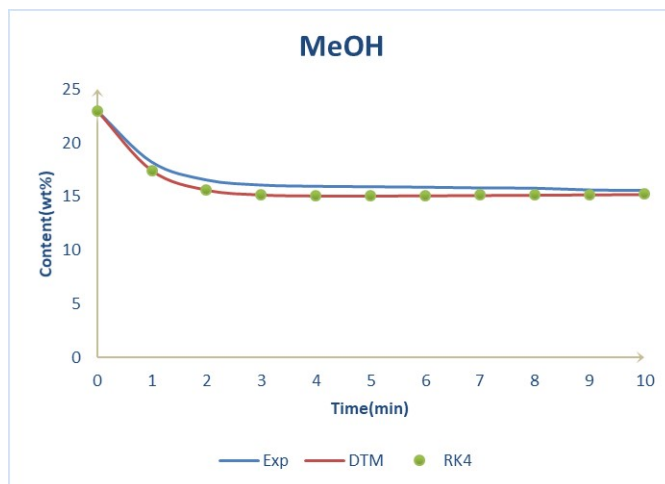


FIGURE 4. Multi-step DTM and RK4 numerical comparisons with experimental results of X_{MeOH} .

TABLE 5. Multi-step DTM and RK4 numerical comparisons with experimental results of X_{MeOH} .

t	$X_{MeOH,DTM}$	$X_{MeOH,RK4}$	$X_{MeOH,exp.}$
0	23	23	23
1	17.44057	17.43994	18.18532
2	15.6316	15.63225	16.5054
3	15.17521	15.17558	16.0331
4	15.07588	15.07603	15.9136
5	15.07214	15.07221	15.8758
6	15.09374	15.09377	15.8294
7	15.12187	15.12189	15.765
8	15.15159	15.1516	15.7365
9	15.1816	15.18161	15.5697
10	15.21157	15.21159	15.52365



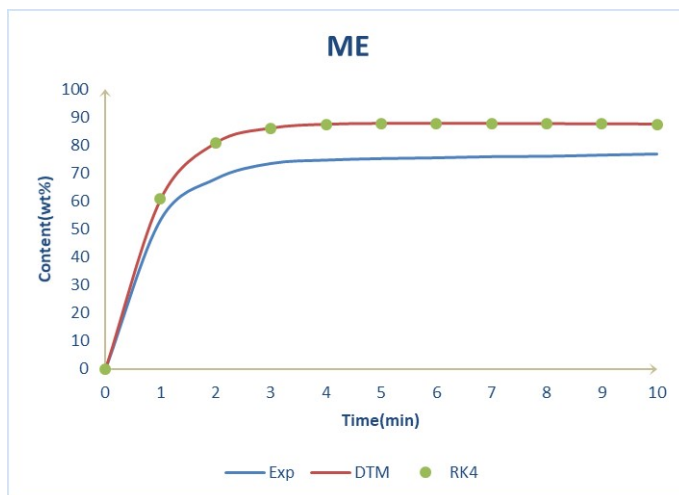


FIGURE 5. Multi-step DTM and RK4 numerical comparisons with experimental results of X_{ME} .

TABLE 6. Multi-step DTM and RK4 numerical comparisons with experimental results of X_{ME} .

t	$X_{ME,DTM}$	$X_{ME,RK4}$	$X_{ME,exp.}$
0	0	0	0
1	60.70764	60.71485	53.51
2	80.80365	80.79663	68.1
3	86.07713	86.0732	73.59
4	87.43377	87.43219	74.8
5	87.74031	89.73974	75.33
6	87.7676	87.7674	75.61
7	87.72172	87.72164	76.02
8	87.65704	87.65699	76.15
9	87.58774	87.5877	76.58
10	87.51751	87.51748	76.96



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