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### Performance of 5-stage, 4-stage and specific stochastic Runge-Kutta methods in approximating the solution of stochastic biological model

#### Noor Amalina Nisa Ariffin<sup>1</sup>, Norhayati Rosli<sup>2</sup>, Abdul Rahman Mohd Kasim<sup>3</sup> and Mazma Syahidatul Ayuni Mazlan<sup>4</sup>

Faculty of Computer and Mathematical Sciences, Universiti Teknologi MARA, Pahang Branch, Jengka Campus, Bandar Pusat Jengka, 26400 Bandar Tun Razak, Pahang Centre for Mathematical Sciences, College of Computing and Applied Sciences, Universiti <sup>2,3,4</sup>Centre for Mathematical Sciences, College of Computing & Applied Sciences, Universiti Malaysia Pahang, Lebuhraya Tun Razak, 26300 Gambang, Kuantan, Pahang, Malaysia

<sup>1</sup>E-mail: amalinanisa@uitm.edu.my

Abstract. In recent years, the transition on modelling physical systems via stochastic differential equations (SDEs) has attracted great interest among researchers. This is due to the limitations of ordinary differential equations in presenting the real phenomenon. To the fact that the stochastic models incorporate the random effects that may influence the behaviour of physical systems, SDEs seems to be the best nodel that can be used in assessing those systems. The growing interest among researchers in nodelling the systems via SDEs comes with the rise in the need of numerical methods to approximate the solutions for SDEs. This is because by taking into account the random fluctuations in SDEs resulting to the complexity of finding the exact solution of SDEs. Therefore, it contribute to the increasing number of research to decide on the best numerical approach to solve the systems of SDEs. This paper is devoted to investigate the performance of 5stage stochastic Runge-Kutta (SRK5) with order 2.0, 4-stage stochastic Runge-Kutta (SRK4), specific stochastic Runge-Kutta with order 1.5 (SRKS1.5) and commutative specific stochastic Runge-Kutta with order 1.5 (SRKST2) in approximating the solution of stochastic model in biological system. A comparative study of SRK5, SRK4, SRKS1.5 and SRKST2 nethods will be presented in this paper. The linear SDE nodel and the stochastic model of C Acetobutylicum cell growth will be used to examine the performance of those nethods and the numerical experiment will be conducted. The numerical solutions obtained will be discussed.

#### 1. Introduction

The nature of almost all physical and biological systems can be visualized via mathematical models. Most of previous researchers choose to model the physical and biological system by using ordinary differential equations (ODEs) [1]. However, due to the condition where the behaviour of the systems are subjected to the random effect from environment, it can't be well presented via ODEs. To the fact that the stochastic models incorporate the random effects that may influence the behaviour of those systems, stochastic differential equations (SDEs) is the best and appropriate model that can be used to describe those systems [2]. In 1951, Ito have done a pioneering work where he formulating SDEs by writing the differential equations



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of ODEs in order to represents deterministic part while for the stochastic part the Wiener process have been incorporated [4]. Wiener process is a process that representing the noise named in honour of Robert Wiener. It is a continuous time stochastic process which oftenly called as Brownian motion. This motion is write to represent the noise that may appear in the system and have been perturbed into ODEs which then turned the differential equations into SDEs. To the knowledge that SDEs are randomly perturbed by noise movement which are unpredictable, the complexity in approximating its analytical solutions comes from the presence of the stochastic part which appeared in SDES. Therefore, most of the SDEs cannot be solved analytically and as such, it is inneed for solving these models numerically. Currently, the research interest have been focusing on finding and developing the best numerical integrator for SDEs. [5] claimed that a heuristic adaptation of a deterministic numerical method for solving SDEs is inconsistent. Therefore, it is of high interest to find the most efficient methods that give the best approximate solutions to SDEs. Maruyama became among the earliest researcher who introduces Euler-Maruyama method as a simplest numerical scheme for solving SDEs. In developing this method, the series of Taylor expansion for SDEs have been truncated at its second terms with 0.5 strong order of convergence [4]. In further work, The Milstein scheme have been introduced by [12] with increasing efficiency to 1.0 strong order of convergence. This method also have been derived from the Taylor series expansion of stochastic differential equations. In motivation from the literature where it has been reported that the Runge-Kutta method have known as an efficient tools to find the numerical solutions of ODEs, Burrage in 1999 applying rooted-tree theory and introduced a new class of SRK method for SDEs [3]. In [7], the method known as Stochastic Runge-Kutta method of stage 4 (SRK4) with order of convergence 1.5 have been developed. As the accuracy order for this SRK method increase, the process of derivation for this method become more complex. Its due to the rapid increasing in the number of equations that need to be worked on for the order condition analysis purposed. Subsequently, the specific SRK (SRKS) with variety of internal stages have been proposed by [9] as the improvement of previous SRK method. It shown that, the complexity presence when dealing with SRK methods of the higher order for SDEs can be reduced by applying the independent internal stages. This will result in the improvement of computation time as well. The latest improvement for SRK method for SDEs have been done by developing the SRK5 with strong order of convergence 2.0 as in [13]. Heretofore, the study on developing the numerical tools for solving SDEs has been increasing rapidly as in [5], [6], [7], [8], [9] and [10]. This paper focusing on examining the performance of SRK5, SRK4 and SRKS as numerical tools to solve the model of stochastic differential equations that exists in biological system. The organization of this research paper are as follows: all methods which are SRKS, SRK5 and SRK4 used in this study will be presented in the next section. Then we considered the stochastic models in biological systems to be solved via those methods. In the next section, the numerical experiment is then performed by applying all numerical methods to find the numerical solutions of all models. The discussion of all results together with the concluding remarks will be devoted in the last section.

## 2. Stochastic Runge-Kutta (SRK) for solving Stochastic Differential Equations(SDEs)

As in [6], SRK4 method has been written generally as follow

$$X_{i}(t) = X_{n}(t_{0}) + h \sum_{j=1}^{i-1} a_{ij}f(x_{j}(t)) + \sum_{j=1}^{i-1} (b_{ij}{}^{(1)}J_{1} + b_{ij}{}^{(2)}\frac{J_{10}}{h})g(x_{j}(t))$$

$$x_{n+1}(t) = x_{n} + h \sum_{j=1}^{s} \alpha_{j}f(x_{j}(t)) + \sum_{j=1}^{s} (\gamma_{j}{}^{(1)}J_{1} + \gamma_{j}{}^{(2)}\frac{J_{10}}{h})g(x_{j}(t))$$
(1)

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where i = 1, ..., s is the stage incorporated in the method.

#### 2.1. 5-stage Stochastic Runge-Kutta with high order of convergence 2.0

In 2018, [13] has developed SRK5 method with 2.0 order of convergence. The scheme of SRK5 can be presented as follows:

$$\begin{aligned} x_{n+1}(t) &= x_n(t_0) + h\alpha_1 f(X_1) + h\alpha_2 f(X_2) + h\alpha_3 f(X_3) + h\alpha_4 f(X_4) + h\alpha_5 f(X_5) \\ &+ (\gamma_1^{(1)} J_1 + \gamma_1^{(2)} \frac{J_{10}}{h}) g(X_1) + (\gamma_2^{(1)} J_1 + \gamma_2^{(2)} \frac{J_{10}}{h}) g(X_2) \\ &+ (\gamma_3^{(1)} J_1 + \gamma_3^{(2)} \frac{J_{10}}{h}) g(X_3) + (\gamma_4^{(1)} J_1 + \gamma_4^{(2)} \frac{J_{10}}{h}) g(X_4) \\ &+ (\gamma_5^{(1)} J_1 + \gamma_5^{(2)} \frac{J_{10}}{h}) g(X_5) \end{aligned}$$
(2)

where

$$\begin{split} X_{1} &= X_{0}^{(n)} \\ X_{2} &= X_{0}^{(n)} + ha_{21}f(X_{1}^{(n)}) + \left(b_{21}^{(1)}J_{1} + b_{21}^{(2)}\frac{J_{10}}{\Delta}\right)g(X_{2}^{(n)}) \\ X_{3} &= X_{0}^{(n)} + ha_{31}f(X_{1}^{(n)}) + ha_{32}f(X_{2}^{(n)}) \\ &+ \left(b_{31}^{(1)}J_{1} + b_{31}^{(2)}\frac{J_{10}}{h}\right)g(X_{1}^{(n)}) + \left(b_{32}^{(1)}J_{1} + b_{32}^{(2)}\frac{J_{10}}{h}\right)g(Y_{2}^{(n)}) \\ X_{4} &= X_{0}^{(n)} + ha_{41}f(X_{1}^{(n)}) + ha_{42}f(X_{2}^{(n)}) + ha_{43}f(X_{3}^{(n)}) \\ &+ \left(b_{41}^{(1)}J_{1} + b_{41}^{(2)}\frac{J_{10}}{h}\right)g(X_{1}^{(n)}) + \left(b_{42}^{(1)}J_{1} + b_{42}^{(2)}\frac{J_{10}}{h}\right)g(X_{2}^{(n)}) \\ &+ \left(b_{43}^{(1)}J_{1} + b_{43}^{(2)}\frac{J_{10}}{h}\right)g(X_{3}^{(n)}) \\ X_{5} &= X_{0}^{(n)} + ha_{51}f(X_{1}^{(n)}) + ha_{52}f(X_{2}^{(n)}) + ha_{53}f(X_{3}^{(n)}) + ha_{54}f(X_{4}^{(n)}) \\ &+ \left(b_{51}^{(1)}J_{1} + b_{51}^{(2)}\frac{J_{10}}{h}\right)g(X_{1}^{(n)}) + \left(b_{52}^{(1)}J_{1} + b_{52}^{(2)}\frac{J_{10}}{h}\right)g(X_{2}^{(n)}) \\ &+ \left(b_{53}^{(1)}J_{1} + b_{53}^{(2)}\frac{J_{10}}{h}\right)g(X_{3}^{(n)}) + \left(b_{54}^{(1)}J_{1} + b_{54}^{(2)}\frac{J_{10}}{h}\right)g(X_{4}^{(n)}) \end{split}$$

In Butcher's tableau form, the numerical scheme of SRK5 method can be written as below

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2.2. 4-stage Stochastic Runge-Kutta with high order of convergence 1.5

SRK4 method have been developed with the 1.5 strong order of convergence based on the formulation (1) written by [3]. The numerical scheme can be written as

$$x_{n+1}(t) = x_n(t_0) + h\alpha_1 f(X_1) + h\alpha_2 f(X_2) + h\alpha_3 f(X_3) + h\alpha_4 f(X_4) + (\gamma_1^{(1)} J_1 + \gamma_1^{(2)} \frac{J_{10}}{h}) g(X_1) + (\gamma_2^{(1)} J_1 + \gamma_2^{(2)} \frac{J_{10}}{h}) g(X_2) + (\gamma_3^{(1)} J_1 + \gamma_3^{(2)} \frac{J_{10}}{h}) g(X_3) + (\gamma_4^{(1)} J_1 + \gamma_4^{(2)} \frac{J_{10}}{h}) g(X_4)$$
(3)

where

$$\begin{split} X_1 &= X_0^{(n)} \\ X_2 &= X_0^{(n)} + ha_{21}f(X_1^{(n)}) + \left(b_{21}^{(1)}J_1 + b_{21}^{(2)}\frac{J_{10}}{h}\right)g(X_1^{(n)}) \\ X_3 &= X_0^{(n)} + ha_{31}f(X_1^{(n)}) + ha_{32}f(X_2^{(n)}) \\ &+ \left(b_{31}^{(1)}J_1 + b_{31}^{(2)}\frac{J_{10}}{h}\right)g(X_1^{(n)}) + \left(b_{32}^{(1)}J_1 + b_{32}^{(2)}\frac{J_{10}}{h}\right)g(X_2^{(n)}) \\ X_4 &= X_0^{(n)} + ha_{41}f(X_1^{(n)}) + ha_{42}f(X_2^{(n)}) + ha_{43}f(X_3^{(n)}) \\ &+ \left(b_{41}^{(1)}J_1 + b_{41}^{(2)}\frac{J_{10}}{h}\right)g(X_1^{(n)}) + \left(b_{42}^{(1)}J_1 + b_{42}^{(2)}\frac{J_{10}}{h}\right)g(X_2^{(n)}) \\ &+ \left(b_{43}^{(1)}J_1 + b_{43}^{(2)}\frac{J_{10}}{h}\right)g(X_3^{(n)}) \end{split}$$

For SRK4 method, its numerical scheme can be presented in the form of Butcher's tableau as below

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#### 2.3. Specific Explicit Stochastic Runge-Kutta method with order 1.5(SRKS)

SRK method (1) cannot be solved easily as it suffer from the complexity for constructing the order conditions due to the large numbers of equations need to be solved. Aiguo & Xioa [9] overcome the withdrawal by introducing a new explicit SRK method together with the introduction to the several groups of independent internal stages. The new specific SRK schemes with 1.5 order of convergence (SRKS 1.5) has been presented. The general form of independent *s*-stage specific SRK method is given by

$$X_{i_{0}}^{0}(t) = X_{n}(t_{0}) + h \sum_{j=1}^{s_{0}} a_{i_{0}j}^{(0)} f(x_{j}^{(0)}(t)) + J_{1} \sum_{j=1}^{s_{0}} b_{i_{0}j}^{(0)} g(x_{j}^{(0)}(t)) \qquad i_{0} = 1, 2, ..., s_{0}$$

$$X_{i_{1}}^{1}(t) = X_{n}(t_{0}) + h \sum_{j=1}^{s_{1}} a_{i_{1}j}^{(1)} f(x_{j}^{(1)}(t)) + \frac{J_{10}}{h} \sum_{j=1}^{s_{1}} b_{i_{1}j}^{(1)} g(x_{j}^{(1)}(t)) \qquad i_{1} = 1, 2, ..., s_{1}$$

$$x_{n+1}(t) = x_{n} + h \sum_{i_{0}=1}^{s_{0}} \alpha_{i_{0}}^{(0)} f(x_{i_{0}}^{(0)}(t)) + J_{1} \sum_{i_{0}=1}^{s_{0}} \gamma_{i_{0}}^{(0)} g(x_{i_{0}}^{(0)}(t)) + h \sum_{i_{1}=1}^{s_{1}} \alpha_{i_{1}}^{(1)} f(x_{i_{1}}^{(1)}(t)) + \frac{J_{10}}{h} \sum_{i_{1}=1}^{s_{1}} \gamma_{i_{1}}^{(1)} g(x_{i_{1}}^{(1)}(t))$$

$$(4)$$

The different internal stages for SRKS method was introduced for the purpose of reducing the number of equations to be solved and been represented by  $s_0$  and  $s_1$ . By letting  $s_0 = 4$  and  $s_1 = 3$ , SRKS 1.5 method was developed yield

$$\begin{aligned} x_{n+1}(t) &= x_n + h(\alpha_1^{(0)} f(x_1^{(0)}(t)) + \alpha_2^{(0)} f(x_2^{(0)}(t)) + \alpha_3^{(0)} f(x_3^{(0)}(t)) + \alpha_4^{(0)} f(x_4^{(0)}(t))) \\ &+ J_1(\gamma_1^{(0)} g(x_1^{(0)}(t)) + \gamma_2^{(0)} g(x_2^{(0)}(t)) + \gamma_3^{(0)} g(x_3^{(0)}(t)) + \gamma_4^{(0)} g(x_4^{(0)}(t))) \\ &+ h(\alpha_1^{(1)} f(x_1^{(1)}(t)) + \alpha_2^{(1)} f(x_2^{(1)}(t)) + \alpha_3^{(1)} f(x_3^{(1)}(t))) \\ &+ \frac{J_{10}}{h}(\gamma_1^{(1)} g(x_1^{(1)}(t)) + \gamma_2^{(1)} g(x_2^{(1)}(t)) + \gamma_3^{(1)} g(x_3^{(1)}(t))) \end{aligned}$$
(5)

with

$$\begin{split} X_1^0(t) &= X_n(t_0) \\ X_2^0(t) &= X_n(t_0) + ha_{21}{}^{(0)}f(x_1^{(0)}(t)) + J_1b_{21}^{(0)}g(x_1^{(0)}(t)) \\ X_3^0(t) &= X_n(t_0) + h(a_{31}{}^{(0)}f(x_1^{(0)}(t)) + a_{32}{}^{(0)}f(x_2^{(0)}(t))) + J_1(b_{31}^{(0)}g(x_1^{(0)}(t)) + b_{32}^{(0)}g(x_2^{(0)}(t))) \\ X_4^0(t) &= X_n(t_0) + h(a_{41}{}^{(0)}f(x_1^{(0)}(t)) + a_{42}{}^{(0)}f(x_2^{(0)}(t)) + a_{43}{}^{(0)}f(x_3^{(0)}(t))) \\ &+ J_1(b_{41}^{(0)}g(x_1^{(0)}(t)) + b_{42}^{(0)}g(x_2^{(0)}(t)) + b_{43}^{(0)}g(x_3^{(0)}(t))) \\ X_1^1(t) &= X_n(t_1) \\ X_2^1(t) &= X_n(t_1) + ha_{21}{}^{(1)}f(x_1^{(1)}(t)) + J_1b_{21}{}^{(1)}g(x_1^{(1)}(t)) \\ X_3^1(t) &= X_n(t_1) + h(a_{31}{}^{(1)}f(x_1^{(1)}(t)) + a_{32}{}^{(1)}f(x_2^{(1)}(t))) + J_1(b_{31}{}^{(1)}g(x_1^{(1)}(t)) + b_{32}{}^{(1)}g(x_2^{(1)}(t))) \end{split}$$

The schemes of SRKS 1.5 can be presented in tableau form as follow

Moreover a general form of SRKS for the SDEs whose drift and diffusion terms are commutative, SRKST2 can be written as

$$X_{i}(t) = X_{n}(t_{0}) + h \sum_{j=1}^{s} a_{ij} f(x_{j}(t)) + J_{1} \sum_{j=1}^{i-1} b_{ij} g(x_{j}(t))$$

$$x_{n+1}(t) = x_{n} + h \sum_{j=1}^{s} \alpha_{j} f(x_{j}(t)) + J_{1} \sum_{j=1}^{s} \gamma_{j}^{(1)} g(x_{j}(t))$$
(6)

for j = 1, ..., s, where s is the stage of SRK method. SRKST2 method can be developed based on (6) and the method is written as

$$x_{n+1}(t) = x_n + \Delta(\alpha_1 f(X_1) + \alpha_2 f(X_2) + \alpha_3 f(X_3) + \alpha_4 f(X_4) + \alpha_5 f(X_5)) + J_1(\gamma_1 g(X_1) + \gamma_2 g(X_2) + \gamma_3 g(X_3) + \gamma_4 g(X_4) + \gamma_5 g(X_5))$$
(7)

where

$$\begin{split} X_1 = & X_n \\ X_2 = & X_n + ha_{21}f(X_1) + J_1b_{21}g(X_1) \\ X_3 = & X_n + h(a_{31}f(X_1) + a_{32}f(X_2)) + J_1(b_{31}g(X_1) + b_{32}g(X_2)) \\ X_4 = & Y_n + h(a_{41}f(X_1) + a_{42}f(X_2) + a_{43}f(X_3)) \\ & + J_1(b_{41}g(X_1) + b_{42}g(X_2) + b_{43}g(X_3)) \\ X_5 = & X_n + h(a_{51}f(X_1) + a_{52}f(X_2) + a_{53}f(X_3) + a_{54}f(X_4)) \\ & + J_1(b_{51}g(X_1) + b_{52}g(X_2) + b_{53}g(X_3) + b_{54}g(X_4)) \end{split}$$

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SRKST2 (7) can be presented in tableu form as



#### 3. Numerical Experiment

In order to analyse the performance of implementations SRK methods to SDE in biological system, the numerical experiment to the linear SDE taken from [10] have been performed. The linear SDE can be considered in the form of

$$dX(t) = aX(t)dt + bX(t)dW(t) \qquad t \in [0,T]$$
(8)

The exact solution of (8) given as

$$X(t) = \exp((a)(t - t_0) + b(W(t) - W(t_0)))(X_0)$$
(9)

Note that we compute this numerical experiment by setting the coefficients as a = -2.0, b = 0.5, T = 2.0, X(0) = 1.0 and h = 0.01. 200 sample paths of strong solutions for SDEs via SRK5, SRK4, SRKS1.5 and SRKST2 have been simulated and the results are presented in Figure 1 and Table 1.

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Figure 1. Exact solution versus numerical solution of (8) via SRK5, SRK4, SRKS1.5 and SRKST2.

Table 1. MSE for SRK5, SRK4, SRKS1.5 and SRKST2.

Numerical Method	SRK5	SRK4	SRKS1.5	SRKST2
MSE	0.007368	0.011736	0.011098	0.031381

Table 2. Global error for SRK5, SRK4, SRKS1.5 and SRKST2.

Numerical Method	SRK5	SRK4	SRKS1.5	SRKST2
Global Error	0.008020	0.016123	0.012198	0.029342

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Figure 1, Table 1 and Table 2 shows the simulated results, mean square error (MSE) and global error respectively for all four methods. All simulated results of SRK5, SRK4, SRKS1.5 and SRKST2 have been compared with the exact solution of the linear SDE (8). From Figure 1, Table 1 and Table 2 presented, it is clearly shown that SRK5 methods provides a solution to the system of linear SDEs that converges to the exact solution. As mentioned in [14], higher order numerical methods will contribute to the efficiency of the method as a tool in solving SDEs. As SRK5 method is the method that have highest order with 2.0 order of convergence, therefore compared to SRK4, SRKS and SRKST2, SRK5 is the most efficient method in approximating the solution to SDEs.

Consider the deterministic model of C. acetobutylicum P262 cell growth as below

$$dx(t) = \mu_{\max} \left( 1 - \frac{x(t)}{x_{\max}} \right) x(t) dt$$

$$x(t_0) = x(0) \qquad t \in [0, T]$$
(10)

x represent the concentration of a cell,  $\mu_{\text{max}}$  represent a growth coefficient and  $x_{\text{max}}$  represent the maximum value of cell growth. The white noise is perturbed to ODE [7] such that

$$b \rightarrow b + \sigma \frac{dW}{dt}$$

where  $b = -\frac{\mu_{\text{max}}}{x_{\text{max}}}$ ,  $\sigma$  is a diffussion coefficient and W(t) is a Wiener process. The stochastic model that incorporated the addition of stochastic process to its deterministic model can be written as below

$$dx(t) = \mu_{\max}\left(1 - \frac{x(t)}{x_{\max}}\right)x(t)dt + \sigma x^2(t)dW(t)$$
(11)

Stochastic model in (11) have been solved viaSRKS1.5, SRKST2, SRK4 and SRK5 methods. We consider the stratonovich form of C. acetobutylicum P262 cell growth model with  $\sigma = 0.0069$ ,  $x_{\text{max}} = 4.565$ ,  $\mu_{\text{max}} = 0.2576$ , and t = 288, with the initial condition y(0) = 0.0025. Cell growth of C. acetobutylicum P262 have been simulated in C++ and the result obtained have been plotted as in Figure 2. The simulated result have been compared to the real data of C. acetobutylicum P262 cell growth and the mean square error and global error obtained have been shown in Table 3 and Table 4 respectively.



**Figure 2**. Experimental data versus numerical solution of (11) via SRK5, SRK4, SRKS1.5 and SRKST2 methods.

Table 3. MSE for SRK5, SRK4, SRKS1.5 and SRKST2.

Numerical Method	SRK5	SRK4	SRKS1.5	SRKST2
MSE	0.20	2.68	0.51	2.80

Table 4. Global error for SRK5, SRK4, SRKS1.5 and SRKST2.

Numerical Method	SRK5	SRK4	SRKS1.5	SRKST2
Global Error	0.873480	0.950640	0.955340	0.959770

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From the results presented above, we can see that the SRK5 method with strong order 2.0 proposed in [13] gives the best result as compared to the real data of cell growth model of C. acetobutylicum P262. The order of convergence of SRK5 proven to be one of the factor that contributes to the efficiency of the numerical method. On the other hand, the computation of the numerical solution of SDEs become more cheaper as a result of the independence internal stages that have been proposed in SRKS methods. From the observation, eventhough SRKST2 method is simpler than SRKS1.5 but because of SRKST2 only evaluate the stochastic integrals  $\frac{J_{10}}{\Delta}$ , hence the SRKST2 gives less efficient result compared to SRKS1.5 method.

#### 4. Conclusion

The random effect or noise that have been corporated in the stochastic model results in complexity of the system increased. Therefore, in this paper four different numerical methods have been used to approximate the numerical solution to the stochastic model. SRK5, SRK4, SRKS1.5 and SRKST2 methods have been used to solve the linear system of SDEs as well as the stochastic model of C. acetobutylicum P262 cell growth. Performance analysis of all methods used have been done in previous section. In conclusion, the highest order of convergence method which is SRK5 have been proven to be the most efficient method and gives better solution compared to SRK4, SRKS1.5 and SRKST2. This method seem to be among the best tools to approximate the solution to the system of SDEs.

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