

ORIGINAL ARTICLE

Numerical Investigation of Auto-Catalytic Glycolysis System Using a Composite Approach Nidhi Prabhakar¹ and Seema Sharma^{2,*}

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Abstract

This paper presents a composite approach which involves forward finite difference, quasi-linearization technique and Haar wavelets to obtain numerical solution of auto-catalytic glycolysis reaction diffusion system with homogeneous Neumann boundary conditions. The time derivative terms present in the system have been approximated using forward finite difference approximation. Nonlinear terms in the system have been linearized using quasi-linearization technique and Haar wavelets have been employed to discretize the space derivatives. To verify the efficiency and accuracy of this approach, numerical simulation is carried out and the obtained solutions have been compared with the solutions given by finite difference scheme. The obtained approximate results validate the well known fact that auto-catalytic glycolysis reaction diffusion system possesses positive solution, as the solutions of auto-catalytic glycolysis reaction diffusion system denote the concentrations of chemical substances. The obtained solutions also satisfy the theory of auto-catalytic glycolysis reaction diffusion system i.e., the steady state solution converges to equilibrium point of auto-catalytic glycolysis reaction diffusion system.

Keywords: Auto-Catalytic Glycolysis Reaction Diffusion System; Forward Finite Difference; Quasi-Linearization; Haar Wavelets

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1. Introduction

Glycolysis is one of the important chemical reactions among all autocatalytic chemical reaction diffusion systems. Glycolysis is a metabolic pathway for converting glucose into pyruvate for energy production. The glycolysis reaction as a whole can be represented as follows Lehninger et al. (1993):

 $C_6H_{12}O_6 + 2NAD^+ + 2ADP + 2P_i \rightarrow 2CH_3COCOO^- + 2NADH + 2H^+ + 2ATP + 2H_2O$

Differential equations are applied in a wide variety of science and engineering fields (Sharma et al. (2010); Delkhosh et al. (2021); Pandit and Sharma (2022); Roul and Kumari (2022)). Various models of chemical reactions in the field of chemistry can be modeled by differential equations. Consequently, researchers are actively engaged in mathematical modeling of such reactions and finding numerical solutions of these models. A simple model of oscillations occurring in glycolysis process was proposed by Sel'kov (1968). The dimensionless form of this model has been given by Strogatz (1994) as

$$\left. \begin{array}{c} \frac{du}{dt} = -u + \sigma_1 v + u^2 v \\ \frac{dv}{dt} = \sigma_2 - \sigma_1 v - u^2 v \end{array} \right\},$$
(1)

where, σ_1 and σ_2 are constant concentrations during the reaction process and are positive kinetic parameters. In coupled system of equation (1), the time dependent variables u and v can have only non-negative values, since they denote the chemical concentration. In his study, Strogatz (1994) demonstrated that this glycolysis system has the fixed point as

$$\begin{pmatrix} u^*, v^* \end{pmatrix} = \left(\sigma_2, \frac{\sigma_2}{\sigma_1 + \sigma_2^2} \right)$$

and the stability condition of fixed point of the glycolysis system is

$$\eta = -\frac{{\sigma_2}^4 + (2\sigma_1 - 1)\sigma_2^2 + (\sigma_1 + {\sigma_1}^2)}{\sigma_1 + \sigma_2^2} < 0.$$

Mickens (2003) applied nonstandard finite difference (NSFD) scheme to solve system (1) numerically and the solution preserved positivity property.

Introducing diffusion in system (1), Zhou and Shi (2015) investigated a general glycolysis reaction diffusion system given by