

Application of Differential Geometry on a Chemical Dynamical Model via Flow Curvature Method

A. K. M. Nazimuddin

Department of Mathematical and Physical Sciences, East West University, Dhaka-1212, Bangladesh
E-mail: nazimuddin@ewubd.edu

Md. Showkat Ali

Department of Applied Mathematics, University of Dhaka, Dhaka-1000, Bangladesh

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Abstract: Slow invariant manifolds can contribute major rules in many slow-fast dynamical systems. This slow manifold can be obtained by eliminating the fast mode from the slow-fast system and allows us to reduce the dimension of the system where the asymptotic dynamics of the system occurs on that slow manifold and a low dimensional slow invariant manifold can reduce the computational cost. This article considers a trimolecular chemical dynamical Brusselator model of the mixture of two components that represents a chemical reaction-diffusion system. We convert this system of two-dimensional partial differential equations into four-dimensional ordinary differential equations by considering the new wave variable and obtain a new system of chemical Brusselator flow model. We observe that the onset of the chemical instability does not depend on the flow rate. We particularly study the slow manifold of the four-dimensional Brusselator flow model at zero flow speed. We apply the flow curvature method to the dynamical Brusselator flow model and acquire the analytical equation of the flow curvature manifold. Then we prove the invariance of this slow manifold equation with respect to the flow by using the Darboux invariance theorem. Finally, we find the osculating plane equation by using the flow curvature manifold.

Index Terms: Trimolecular Flow Model, Slow Manifold, Flow Curvature Method, Invariance Property.

1. Introduction

Many dynamical systems contain slow-fast structure where the dynamics of the system goes slowly but towards the slow invariant manifold, the trajectory of the system from any initial point rapidly relaxes. Slow invariant manifolds can exist in singularly as well as non-singularly perturbed systems [1, 2, 3]. To obtain the equation of the slow manifold, the classical Geometric Singular Perturbation (GSP) technique [4, 5, 6, 7] is one of the techniques among various methods which use asymptotic expansion and this technique is applicable only for a singularly perturbed dynamical system. Another new method to determine the equation of slow manifold is the Flow Curvature Method (FCM) [8, 9, 10, 11, 12] and this method is applicable for a system whether it is a singularly perturbed dynamical system or not. Ginoux and Rossetto [13] adopted this FCM to the heartbeat model to generate the slow invariant manifold equation. Using the FCM, Ginoux [14] determined the equation of the slow manifold of the L-K model.

Angelov and Stoltz analyzed the asymptotic solution behavior of the Brusselator chemical dynamical model [15]. Different and interesting types of pattern formation induced from the Brusselator model through the numerical investigation are observed in [16]. Using the numerical bifurcation analysis, solutions of Periodic traveling waves and their stability of the Brusselator model are investigated in [17, 18]. Recently, the FCM was used to determine the equation of the slow manifold of the Brusselator chemical dynamical model [19].

The main research objective of this article is to find the analytical equation of the slow invariant manifold of the Brusselator flow model at zero speed. We have used a differential geometry-based method, namely FCM that is best because this method can be applied on both singularly perturbed systems and non-singularly perturbed systems and does not use the asymptotic expansion technique. In this article, we consider a two-dimensional dynamical Brusselator model. The reaction-diffusion Brusselator prepares a useful model for the study of cooperative processes in chemical kinetics, such as trimolecular reaction steps arising from the formation of ozone by atomic oxygen via a triple collision. This system also governs in enzymatic reactions and in plasma and laser physics in multiple couplings between certain modes. We convert this system of two-dimensional partial differential equations into four-dimensional ordinary

differential equations. We set a new wave variable so that our new four-dimensional dynamical model can be regarded as a flow model. We apply the differential geometry-based FCM to the dynamical four-dimensional Brusselator flow model and obtain the analytical equation of the flow curvature manifold. After that, we use the Darboux invariance theorem to prove the invariance of the slow manifold with respect to the flow. We also find the osculating plane equation by using the flow curvature manifold.

The rest part of this article is organized as follows. The Brusselator flow model is described in section 2. In section 3, we discuss a differential geometry based flow curvature method. Analysis of flow curvature manifold in the Trimolecular Brusselator flow model is discussed in section 4. The osculating plane equation using flow curvature manifold is also described in section 5. In section 6, we give some concluding remarks and discussions related to this article.

2. Trimolecular Brusselator Flow Model

The Trimolecular model or Brusselator system describes the following chemical reactions [20]. The the chemical Brusselator model in dimensionless form can be written as follows:

$$\begin{aligned}\frac{\partial U}{\partial t} &= D\Delta U + A - (B+1)U + U^2 V, \\ \frac{\partial V}{\partial t} &= \Delta V + BU - U^2 V.\end{aligned}\tag{1}$$

where the dimensionless concentrations are U and V called activator and inhibitor, respectively and the kinetic parameters are A and B and the diffusion coefficient is D .

We consider $z = x - Ct$ where z is the traveling wave coordinate, C is the wave speed and also x and t are the space and time coordinates, respectively. By substituting $U(x, t) = u(z)$ and $V(x, t) = v(z)$ in our model (1), we get the wave equations as follows:

$$\begin{aligned}D\frac{d^2u}{dz^2} + C\frac{du}{dz} + A - (B+1)u + u^2v &= 0, \\ \frac{d^2v}{dz^2} + c\frac{dv}{dz} + Bu - u^2v &= 0.\end{aligned}$$

Now we can write the above system as a set of four-dimensional ordinary differential equations as the following:

$$\begin{aligned}\frac{du}{dz} &= p, \\ \frac{dp}{dz} &= (-Cp - A + (B+1)u - u^2v)/D, \\ \frac{dv}{dz} &= q, \\ \frac{dq}{dz} &= -Cq - Bu + u^2v.\end{aligned}\tag{2}$$

3. Flow Curvature Method

In this part, we briefly discuss the flow curvature method in terms of differential geometry. This method uses the properties of curvatures of trajectory curve or flow of the dynamical system. Using this method, one can define the flow curvature manifold corresponding to the dynamical system. Any n -dimensional dynamical system can have the $(n-1)$ dimensional flow curvature manifold that means flow curvature manifold contains the information about the flow with highest curvature.

Invariant manifold implies a very significant role to explain the stability as well as dynamical behavior of a system, especially for a slow-fast dynamical system. Although geometric perturbation technique is well known to find the analytical equation of slow manifold, the main difference between geometric perturbation technique and the flow

curvature method is that it neither uses asymptotic expansions nor eigenvectors. Another difference is that this method can be used for any dynamical system which may or may not singularly perturbed.

Proposition 3.1 The set of points where the curvature of the flow vanishes represented by the following flow curvature manifold equation of the dynamical system.

$$\psi(\vec{X}) = \det(\vec{X}, \vec{X}) = 0$$

Proof See [9,10]

Note that for any n-dimensional dynamical system, maximum (n-1)th flow curvature is possible.

Proposition 3.2 The flow curvature manifold of the dynamical system (1) directly provides its implicit analytical equation of the slow manifold.

Proof See [9,10]

4. Brusselator Flow Model Analysis Using FCM

According to the FCM, this method is applicable for a system whether it is a singularly perturbed dynamical system or not. We consider the chemical Brusselator flow model (2) as a slow-fast dynamical system.

The velocity vector of the flow model (2) is as follows

$$\vec{V} = \left\{ p, \frac{-A - cp + (1+B)u - u^2v}{D}, q, -cq - Bu + u^2v \right\}$$

We obtain the following single fixed point of the system (2).

$$u_1 = A, p_1 = 0, v_1 = \frac{B}{A}, q_1 = 0$$

The following is the Jacobian matrix at the fixed point for the model (2)

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ \frac{1+B-2uv}{D} & -4c & -4u^2 & 0 \\ 0 & 0 & 0 & 1 \\ -B+2uv & 0 & u^2 & -c \end{pmatrix}$$

Table 1. Assumed parameter values of the model (2)

| Parameters | A | B | C | D |
|------------|-----|------|---|------|
| Values | 4.0 | 20.0 | 0 | 0.25 |

We use the parameter values of (2) as mentioned in Table 1 indicates the assumed parameter values of the model (2) and we also consider the following ranges of the state variables for the numerical simulations.

$$[u_{\min}, u_{\max}] = [-1000, 1000];$$

$$[p_{\min}, p_{\max}] = [-1000, 1000];$$

$$[v_{\min}, v_{\max}] = [-1000, 1000];$$

We obtain the following single fixed point of the system (2).

$$u_1 = 4.0, p_1 = 0, v_1 = 5.0, q_1 = 0$$

The following is the Jacobian matrix at the fixed point for the model (2)

$$J = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 84 - 8uv & 0 & -4u^2 & 0 \\ 0 & 0 & 0 & 1 \\ -20 + 2uv & 0 & u^2 & 0 \end{pmatrix}$$

The eigenvalues of the above Jacobian matrix corresponding to the model (2) at the fixed point can be written as

$$\{-9.16515, 0, 0, 9.16515\}$$

We apply the fourth order Runge-Kutta method in order to solve the flow model (2), where we consider $(u_0, p_0, v_0, q_0) = (4.1, 0, 5.1, 0)$ as an initial point. A three-dimensional graphical behaviour of the phase plot shown in Fig.1, where t ranges from 0 to 100. We numerically calculate three dimensional parametric plot of u, p, v , where t ranges from 20 to 70. The green point in the Fig.1 indicate the fixed point of the model (2).

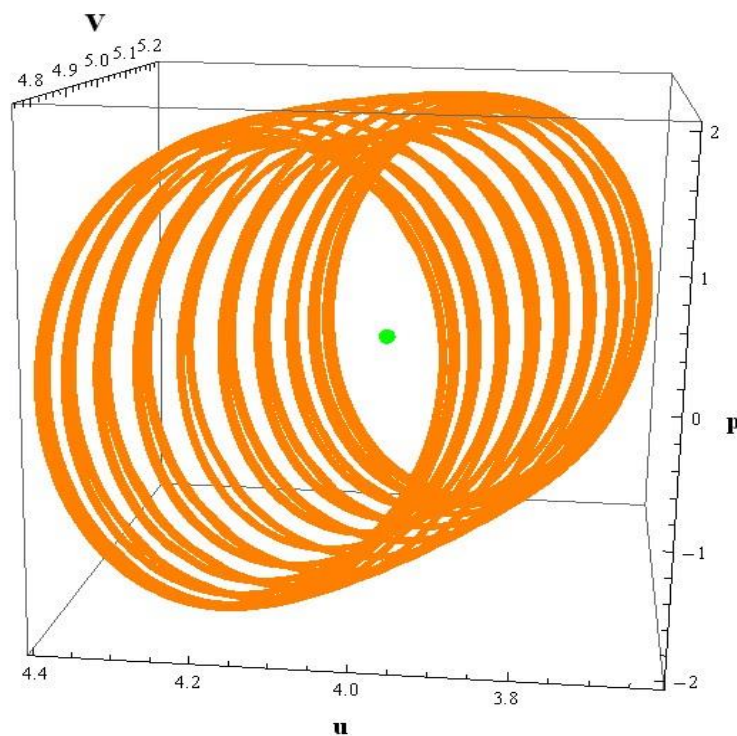


Fig.1. Three-dimensional Phase plot analysis for the model (2) along with the single fixed point.

We present two-dimensional parameter plots using the numerical simulation of model (2), where t ranges from 0 to 70. Fig.2a shows the graph of u and p which reflects the closed region represented by the red color, fig.2b shows the graph of u and v which reflects the closed region represented by the green color, fig.2c shows the graph of p and v which reflects the closed region represented by the blue color and Fig.2d shows the graph of u and q which reflects the closed region represented by the cyan color. Fig.2a, fig.2b, fig.2c and fig.2d also represents periodic solution of the model (2).

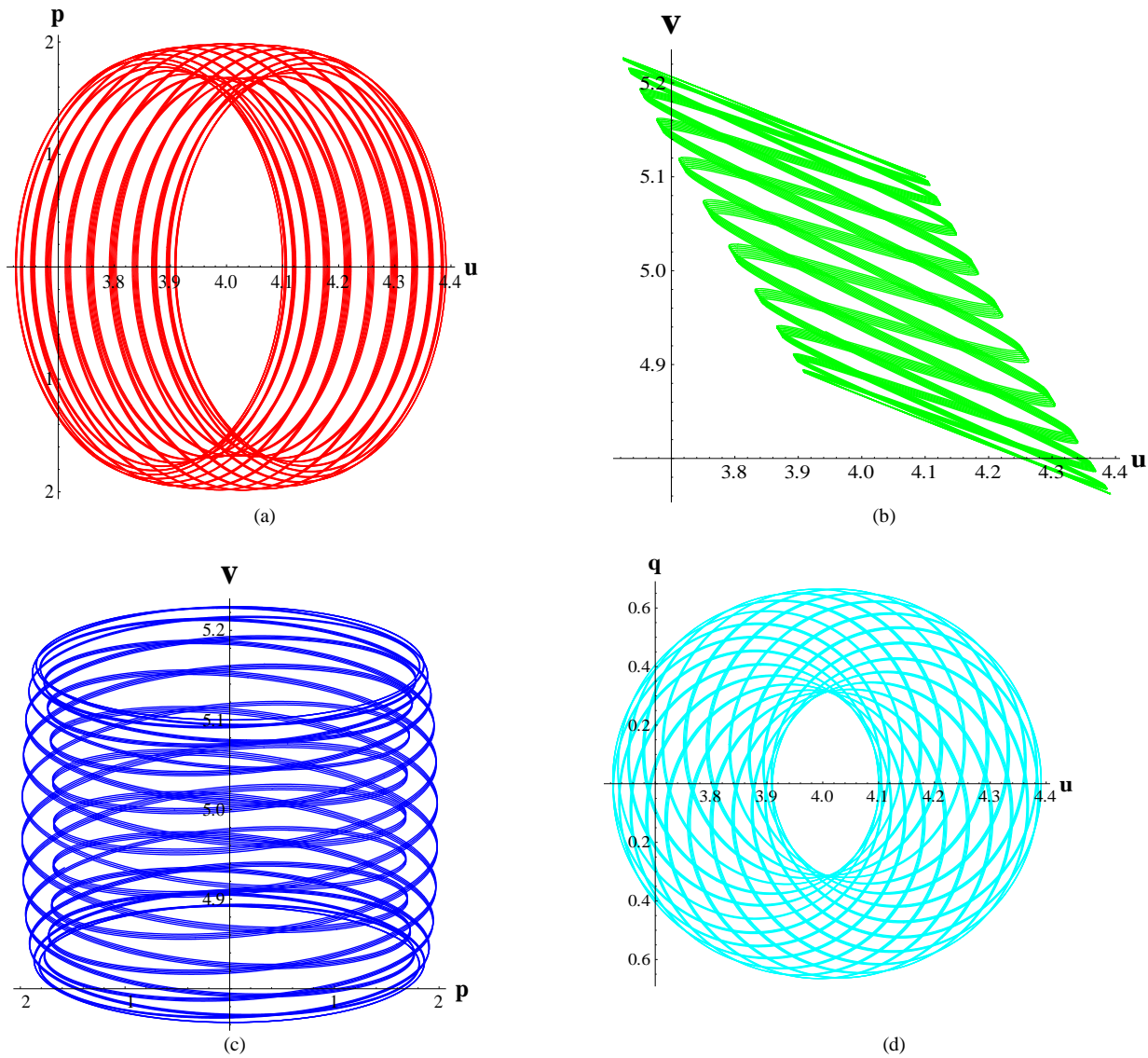


Fig.2. (a) Graphical representation of u and p , (b) Graphical representation of u and v , (c) Graphical representation of p and v , (d) Graphical representation of u and q .

Now according to the FCM, we first calculate the velocity vector, acceleration vector, over-acceleration vector (Jerk) and over-jerk because of our 4-dimensional dynamical model.

The velocity vector of the flow model (2) is as follows

$$\vec{V}_1 = \{p, 4(-4 + 21u - u^2v), q, -20u + u^2v\}$$

By using the formula $\vec{V}_2 = J\vec{V}_1$, we can write the acceleration vector as the following

$$\begin{aligned} \vec{V}_2 = \{ & 4(-4 + 21u - u^2v), 0 - 4qu^2 + p(84 - 8uv), \\ & 0 - 20u + u^2v, 0 + qu^2 + p(-20 + 2uv) \} \end{aligned}$$

Now, the over-acceleration vector or jerk vector is expressed using a equation $\vec{V}_3 = J\vec{V}_2$ and then, we obtain

$$\begin{aligned} \vec{V}_3 = \{ & 0 - 4qu^2 + p(84 - 8uv), 4(84 - 8uv)(-4 + 21u - u^2v) - 4u^2(0 - 20u + u^2v), \\ & 0 + qu^2 + p(-20 + 2uv), 4(-20 + 2uv)(-4 + 21u - u^2v) + u^2(0 - 20u + u^2v) \} \end{aligned}$$

Then, the over- jerk vector is expressed using a equation $\vec{V}_4 = J\vec{V}_3$ and hence, we obtain

$$\vec{V}_4 = \{4(84 - 8uv)(-4 + 21u - u^2v) - 4u^2(0 - 20u + u^2v), (84 - 8uv)(0 - 4qu^2 + p(84 - 8uv)) - 4u^2(0 + qu^2 + p(-20 + 2uv)), 4(-20 + 2uv)(-4 + 21u - u^2v) + u^2(0 - 20u + u^2v), (-20 + 2uv)(0 - 4qu^2 + p(84 - 8uv)) + u^2(0 + qu^2 + p(-20 + 2uv))\}$$

By assuming $q \rightarrow 0$, we can express the slow manifold function is as follows

$$\phi(u, p, v) = 16 \left(\begin{aligned} &1.6384 \times 10^6 - 537600 p^2 - 1.72032 \times 10^7 u + 4.51584 \times 10^7 u^2 - 6400 p^2 u^2 + 100 p^4 u^2 \\ &- 204800 u^3 + 6400 p^2 u^3 + 1.1264 \times 10^6 u^4 - 8400 p^2 u^4 - 268800 u^5 + 6400 u^6 - 100 p^2 u^6 \\ &- 3200 u^7 + 400 u^8 - 327680 uv + 158720 p^2 uv + 4.3008 \times 10^6 u^2 v - 13440 p^2 u^2 v \\ &- 1.37626 \times 10^7 u^3 v + 1280 p^2 u^3 v - 20 p^4 u^3 v + 1.15968 \times 10^6 u^4 v - 1120 p^2 u^4 v - 222720 u^5 v \\ &+ 1720 p^2 u^5 v + 67200 u^6 v - 4000 u^7 v + 10 p^2 u^7 v + 320 u^8 v - 40 u^9 v + 16384 u^2 v^2 - 15616 p^2 u^2 v^2 \\ &- 339968 u^3 v^2 + 2624 p^2 u^3 v^2 + 1.47789 \times 10^6 u^4 v^2 - 148 p^2 u^4 v^2 + p^4 u^4 v^2 - 224128 u^5 v^2 + 48 p^2 u^5 v^2 \\ &+ 20496 u^6 v^2 - 106 p^2 u^6 v^2 - 4608 u^7 v^2 + 344 u^8 v^2 - 0.25 p^2 u^8 v^2 - 8 u^9 v^2 + u^{10} v^2 + 512 p^2 u^3 v^3 \\ &+ 8192 u^4 v^3 - 128 p^2 u^4 v^3 - 65536 u^5 v^3 + 8 p^2 u^5 v^3 + 13440 u^6 v^3 - 928 u^7 v^3 + 2 p^2 u^7 v^3 + 96 u^8 v^3 \\ &- 8 u^9 v^3 + 1024 u^6 v^4 - 256 u^7 v^4 + 16 u^8 v^4 \end{aligned} \right)$$

Now the equation of the slow manifold of the model (2) is as follows

$$\phi(u, p, v) = 0 \quad (3)$$

Three dimensional graphical illustration of the slow manifold of the model (2) that is represented by the equation (3) which shows in Fig.3(a). Three dimensional graphical illustration of the slow manifold along with the phase diagram shows in Fig.3(b).

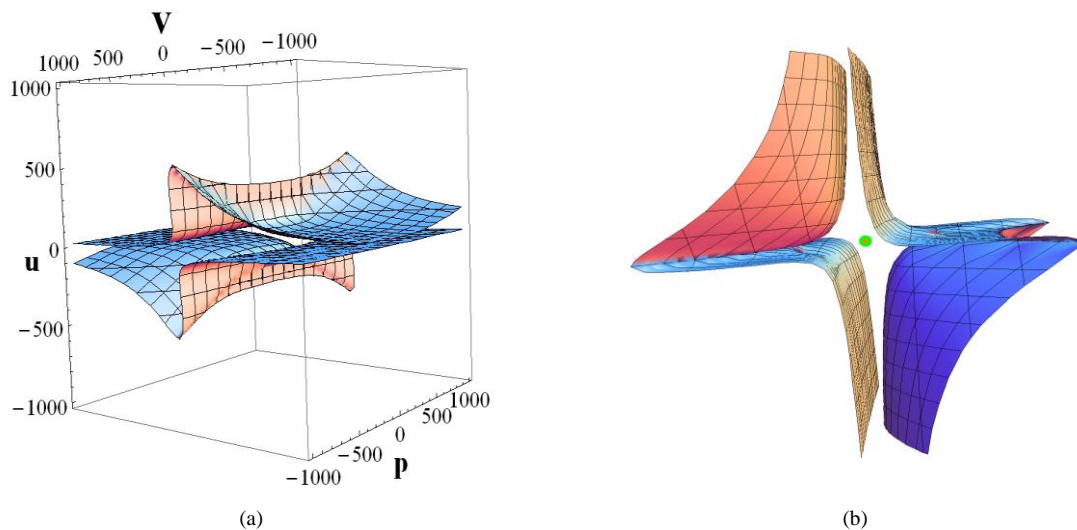


Fig.3. (a) Three dimensional graphical illustration of the slow manifold of the model (2) (b) Three dimensional graphical illustration of the slow manifold along with the phase diagram.

First we determine the normal vector on the flow curvature manifold. Then using this normal vector we can find the Lie derivative by using the Darboux theory.

$$\begin{aligned}\bar{\nabla}\phi = & \{16(-1.72032 \times 10^7 + 9.03168 \times 10^7 u - 12800 p^2 u + 200 p^4 u - 614400 u^2 \\ & + 19200 p^2 u^2 + 4.5056 \times 10^6 u^3 - 33600 p^2 u^3 - 1.344 \times 10^6 u^4 + 38400 u^5 - 600 p^2 u^5 \\ & - 22400 u^6 + 3200 u^7 - 327680 v + 158720 p^2 v + 8.6016 \times 10^6 uv - 26880 p^2 uv \\ & - 4.12877 \times 10^7 u^2 v + 3840 p^2 u^2 v - 60 p^4 u^2 v + 4.63872 \times 10^6 u^3 v - 4480 p^2 u^3 v \\ & - 1.1136 \times 10^6 u^4 v + 8600 p^2 u^4 v + 403200 u^5 v - 28000 u^6 v + 70 p^2 u^6 v + 2560 u^7 v \\ & - 360 u^8 v + 32768 uv^2 - 31232. p^2 uv^2 - 1.0199 \times 10^6 u^2 v^2 + 7872 p^2 u^2 v^2 \\ & + 5.91155 \times 10^6 u^3 v^2 - 592. p^2 u^3 v^2 + 4. p^4 u^3 v^2 - 1.12064 \times 10^6 u^4 v^2 + 240 p^2 u^4 v^2 \\ & + 122976 u^5 v^2 - 636 p^2 u^5 v^2 - 32256 u^6 v^2 + 2752 u^7 v^2 - 2 p^2 u^7 v^2 - 72 u^8 v^2 + 10 u^9 v^2 \\ & + 1536 p^2 u^2 v^3 + 32768 u^3 v^3 - 512 p^2 u^3 v^3 - 327680 u^4 v^3 + 40 p^2 u^4 v^3 + 80640 u^5 v^3 \\ & - 6496 u^6 v^3 + 14 p^2 u^6 v^3 + 768 u^7 v^3 - 72 u^8 v^3 + 6144 u^5 v^4 - 1792 u^6 v^4 + 128 u^7 v^4), \\ & 16(-1.0752 \times 10^6 p - 12800 pu^2 + 400 p^3 u^2 + 12800 pu^3 - 16800 pu^4 - 200 pu^6 + 317440 puv \\ & - 26880 pu^2 v + 2560 pu^3 v - 80 p^3 u^3 v - 2240 p u^4 v + 3440 p u^5 v + 20 p u^7 v - 31232 pu^2 v^2 \\ & + 5248 p u^3 v^2 - 296 pu^4 v^2 + 4 p^3 u^4 v^2 + 96 p u^5 v^2 - 212 pu^6 v^2 - 0.5 pu^8 v^2 + 1024 pu^3 v^3 \\ & - 256 pu^4 v^3 + 16 pu^5 v^3 + 4 pu^7 v^3), \\ & 16(-327680 u + 158720 p^2 u + 4.3008 \times 10^6 u^2 - 13440 p^2 u^2 - 1.37626 \times 10^7 u^3 + 1280 p^2 u^3 \\ & - 20 p^4 u^3 + 1.15968 \times 10^6 u^4 - 1120 p^2 u^4 - 222720 u^5 + 1720 p^2 u^5 + 67200 u^6 - 4000 u^7 \\ & + 10 p^2 u^7 + 320 u^8 - 40 u^9 + 32768 u^2 v - 31232 p^2 u^2 v - 679936 u^3 v + 5248 p^2 u^3 v + 2.95578 \times 10^6 u^4 v \\ & - 296 p^2 u^4 v + 2 p^4 u^4 v - 448256 u^5 v + 96 p^2 u^5 v + 40992 u^6 v - 212 p^2 u^6 v - 9216 u^7 v + 688 u^8 v - 0.5 p^2 u^8 v \\ & - 16 u^9 v + 2 u^{10} v + 1536 p^2 u^3 v^2 + 24576 u^4 v^2 - 384 p^2 u^4 v^2 - 196608 u^5 v^2 + 24 p^2 u^5 v^2 + 40320 u^6 v^2 \\ & - 2784 u^7 v^2 + 6 p^2 u^7 v^2 + 288 u^8 v^2 - 24 u^9 v^2 + 4096 u^6 v^3 - 1024 u^7 v^3 + 64 u^8 v^3), \\ & 0\}\end{aligned}$$

Now the Lie derivative of the slow manifold can be written as

$$\mathcal{L}_{\bar{\nabla}}\phi = 32 \begin{pmatrix} -6400 p^3 u + 100 p^5 u - 204800 pu^2 + 6400 p^3 u^2 + 1.6128 \times 10^6 pu^3 - 686400 pu^5 \\ - 300 p^3 u^5 - 9600 pu^6 - 6800 pu^7 - 163840 pv + 79360 p^3 v + 1.76128 \times 10^6 puv \\ - 13440 p^3 uv - 4.94592 \times 10^6 pu^2 v + 1920 p^3 u^2 v - 30 p^5 u^2 v + 1.16992 \times 10^6 pu^3 v \\ - 1600 p^3 u^3 v - 405760 pu^4 v + 140 p^3 u^4 v + 54400 pu^5 v + 164080 pu^6 v + 35 p^3 u^6 v \\ + 1120 pu^7 v + 1060 pu^8 v + 16384 puv^2 - 15616 p^3 uv^2 - 260096 pu^2 v^2 + 3936 p^3 u^2 v^2 \\ + 967168 pu^3 v^2 - 296 p^3 u^3 v^2 + 2. p^5 u^3 v^2 - 283776. pu^4 v^2 + 88 p^3 u^4 v^2 + 43168 p u^5 v^2 \\ + 10 p^3 u^5 v^2 - 5920 pu^6 v^2 - 14408 p u^7 v^2 - p^3 u^7 v^2 - 32 pu^8 v^2 - 56 pu^9 v^2 + 768 p^3 u^2 v^3 \\ + 8192 pu^3 v^3 - 256 p^3 u^3 v^3 - 56320 p u^4 v^3 + 20 p^3 u^4 v^3 + 18944 pu^5 v^3 - 1984 pu^6 v^3 \\ - p^3 u^6 v^3 + 160 p u^7 v^3 + 556 p u^8 v^3 + p u^{10} v^3 + 1024 pu^5 v^4 - 384 pu^6 v^4 + 32 pu^7 v^4 - 8 pu^9 v^4 \end{pmatrix}$$

Fig.4(a) shows a three dimensional graphical illustration of the equation $\mathcal{L}_{\vec{v}}\phi = 0$ that means of the rate of change of the flow curvature manifold $\phi(u, p, v)$ is zero. Three dimensional graphical illustration of the invariance equation of slow manifold along with the phase diagram shows in Fig.4(b).

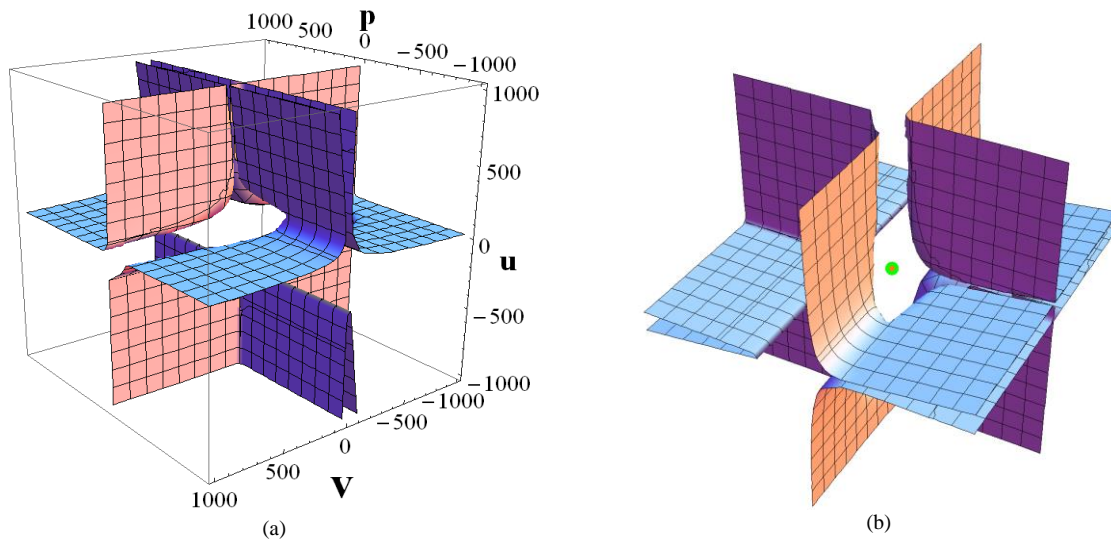


Fig.4. (a) Three dimensional graphical illustration of the invariance equation of slow manifold., (b) Three dimensional graphical illustration of the invariance equation of slow manifold along with the phase diagram.

5. The Equation of Osculating Plane

We determine the equation of the osculating plane for the fixed point $u_1 = 4.0, p_1 = 0, v_1 = 5.0, q_1 = 0$. We get the following osculating plane equation.

$$P(\vec{X}) = -4 \left(\begin{aligned} &102400 - 40000 p^2 + 100 p^4 - 1.1776 \times 10^6 u + 4800 p^2 u + 3.3856 \times 10^6 u^2 \\ &- 8400 p^2 u^2 - 140800 u^3 + 100 p^2 u^3 + 41600 u^4 - 100 p^2 u^5 - 11600 u^5 \\ &+ 400 u^6 - 20480 v + 6720 p^2 + 204800 u v + 7840 p^2 u v - 20 p^4 u v \\ &- 389120 u^2 v - 1300 p^2 u^2 v - 674560 u^3 v + 1680 p^2 u^3 v + 62160 u^4 v \\ &- 5 p^2 u^4 v - 4000 u^5 v + 10 p^2 u^5 v + 1140 u^6 v - 40 u^7 v + 2048 u v^2 \\ &- 1312 p^2 u v^2 - 32000 u^2 v^2 - 300 p^2 u^2 v^2 + p^4 u^2 v^2 + 107264 u^3 v^2 \\ &+ 80 p^2 u^3 v^2 + 33520 u^4 v^2 - 104 p^2 u^4 v^2 - 4992 u^5 v^2 + 96 u^6 v^2 \\ &- 0.25 p^2 u^6 v^2 - 28 u^7 v^2 + u^8 v^2 + 64 p^2 u^2 v^3 + 1024 u^3 v^3 - 8 p^2 u^3 v^3 \\ &- 6784 u^4 v^3 - 96 u^5 v^3 + 2 p^2 u^5 v^3 + 112 u^6 v^3 + 128 u^5 v^4 - 16 u^6 v^4 \end{aligned} \right)$$

Now, a three dimensional graphical behaviour of the equation of the osculating plane represented by $P(\vec{X}) = 0$ is shown in fig. 5.

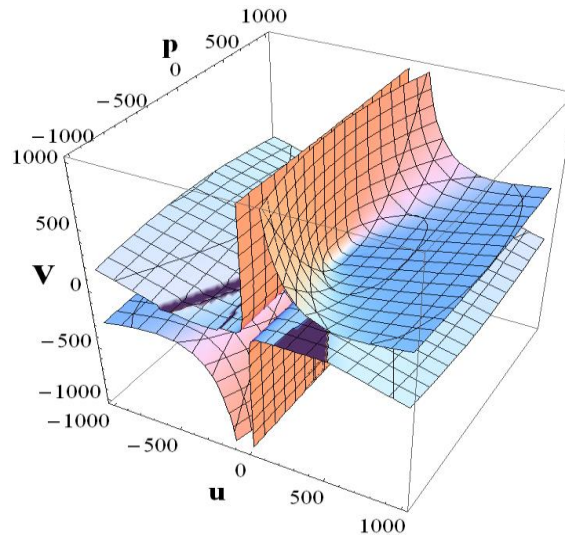


Fig.5. Graph of the osculating plane where we use the fixed point (u_1, p_1, v_1, q_1) .

6. Conclusion

Slow invariant manifolds are very important to acquire the model reduction of a system where the system exhibits spatially non-homogeneous and the phase space of the system is closed. The main concern of this article is to determine the location of a special trajectory, the so-called slow manifold of the flow model. In this paper, we analyzed a two-dimensional dynamical Brusselator model. We converted this system of two-dimensional partial differential equations into four-dimensional ordinary differential equations by considering a new wave variable so that our new four-dimensional dynamical model can be regarded as a flow model. We particularly studied the slow manifold of the four-dimensional Brusselator flow model at zero flow speed for the first time and this study advances the field from the previous related work. We applied the differential geometry-based FCM to the dynamical four-dimensional Brusselator flow model and obtained the analytical equation of the flow curvature manifold. We then used the Darboux invariance theorem to prove the invariance of the slow manifold with respect to the flow. We also established the osculating plane equation by using the flow curvature manifold.

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Authors' Profiles



A. K. M. Nazimuddin received his PhD in Applied Mathematics from the University of Dhaka, Bangladesh. He completed his B. S. (Hon's) in Mathematics and M. S. in Applied Mathematics from the University of Dhaka, Bangladesh. He is now working as an Assistant professor in the Department of Mathematical and Physical Sciences, East West University, Dhaka, Bangladesh. His research interests include Dynamical Systems, Differential Geometry.



Md. Showkat Ali received his PhD from the University of Glasgow, Glasgow, UK. He completed his B. S. (Hon's) degree in Mathematics and M. S. in Applied Mathematics from the University of Dhaka, Bangladesh. Currently, he is working as a Professor and Chairman in the Department of Applied Mathematics, University of Dhaka. His research interests include Differential Geometry and Dynamical Systems.

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