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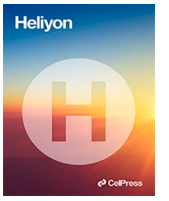

Research article

Numerical and computational analysis on a dissipative dynamical system: Slow invariant manifold for complex chemical mechanism

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ABSTRACT

This article presents the notion about Slow Invariant Manifold (SIM) and their fundamental role in model reduction techniques (MRTs) for challenges encountered in mechanical engineering within dissipative systems of chemical kinetics. Focusing on the reaction routes of complex mechanisms, we construct and compare primary approximations of the SIM through MRTs, including the Spectral Quasi Equilibrium Manifold (SQEM) and Intrinsic Low Dimensional Manifold (ILDM). These methods effectively transform high-dimensional complex problems into lower dimensions, solving them without compromising crucial information about the complex systems modified for homogeneous reactive systems. Employing the sensitivity analysis by using the MATLAB's toolbox, we present the numerical findings in a tabular format obtained through MRTs. This study provides the understanding about the accessible exploration of numerical solutions, improving insights of the complex variation within the system.

1. Introduction

The intricacy of complex mechanisms in chemical kinetics may be increase by huge number of chemical components. To overcome this complexity, the number of elementary reactions that can accurately disclose the formation of complex reaction. In the chemical kinetics, the rate of reactions and the factors that effecting these reaction rates are examined. The biological systems, combustion reactions and in physical chemistry the chemical systems are very complex due to their great number of reactions and chemical species. Moreover, the observation of the complex mechanism is very difficult, time-consuming and costly effecting due to the large computations. Without effecting the efficiency of reaction mechanism, MRTs addressing the major challenges by constructing a reduced models [1–3].

To address these challenges, reduced description approaches generate essential characteristics of the system in the form of simplified models. The quasi steady-state approximation (QSSA) is a technique commonly used in these simplified models, which group together complexity [4,5]. This approach assumes that some species experience slower fluctuations in concentration during the reaction process than other species, and that these species eventually establish a steady state [6]. Another approach is partial equilibrium, which operates on the theory that if some reactions equilibrate quickly compared to others, computations of concentrations

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for associated species can be performed independently [7]. Detailed comparison and analysis of simulations are necessary to validate and enhance these simplified models, ensuring that experimental results are trustworthy and applicable [8].

In chemical kinetics, the problem of limited description is significant. By creating chemical models, investigators can increase perceptions into complex chemical systems and develop more manageable simulations applicable in real-world scenarios. Increased complexity arises from additional steps or species (atoms, molecules, ions). Numerous approaches and strategies have been devised to reduce this complexity [9]. By implementing various model reduction techniques (MRTs) and considering the slow and fast phases of reactions, the complication of the mechanism can be decreased without compromising its inventiveness [10,11]. As reduced species approach equilibrium by completing transitional periods with varying initial conditions, MRTs must explore approximate solution curves in phase-space and trajectories [12–14]. This kind of invariant region, known as a SIM, is crucial for simplifying models [15]. Two essential techniques for analyzing complex interactions with higher dimensions are the SQEM and the ILDM [16–18]. These techniques decompose the model's structure, achieving intended solution qualities without compromising the overall reaction mechanism. The kinetics of reactions and the parameters over different time scales inter into micro and macro level studies [19–23]. Various reaction mechanisms exhibit distinct behaviors based on their composition and nature, necessitating both theoretical and experimental understanding.

Similarly, sensitivity analysis is another technique that measures how input factors affect output variables; for further information, refer to Refs. [24,25]. When the degree of freedom exceeds three dimensions, model reduction becomes necessary. Intermediate species form in one step and are consumed in the next, while non-intermediate species are present in the overall reaction. Complex reactions contain numerous intermediates, terminal species, and elementary steps. Research efforts in this area have focused on understanding and mitigating these factors to refine understanding complex chemical kinetics [16,26]. Moreover, additional techniques, such as sensitivity analysis, exist to quantitatively assess the impression on the output variables of input parameters [27]. Further details regarding these techniques can be found in references [25]. Furthermore, understanding the distribution across multiple routes is very important, particularly when the mathematical model of the reaction system consists of degrees of freedom more than three [26]. Terminal species are directly involved within a complex reaction system, while intermediates are generated through the reaction process but are not engaged in the net reaction [27,28]. Elementary steps in a complex reaction mechanism involve intermediate and terminal species, whereas an overall reaction involves only the terminal species participating [29].

The article is prepared as follows: Section 2 provides the research and presents the model formulation, along with the necessary and sufficient definitions for our task. Here, we develop a kinetic model to ascertain the reaction process, which remains crucial for the overall system. This section covers the overall concept of building the kinetic equations. Section 3 discusses various accessible initial approximation strategies. The reduced system will be simulated to maintain the accuracy of the entire mechanism, using the reduced form of the data obtained via the approximation techniques. Section 4 addresses the complex reaction problem. Section 5 discusses the outcomes and comparisons.

The main objective of this study is to compare the solution behavior of chemical species obtained through different model reduction techniques to translate the difficulty in the multi-step reaction. Also, the sensitivity analysis allows us to differentiate the sensitivity of the chemical species.

2. Mathematical modelling

2.1. Kinetic equations and MRTs

When the reactions reached at equilibrium state, then with several elementary steps mechanism of reversible reaction is given as in equation (1):

$$\sum_{j=1}^{n} r_j A_j \Leftrightarrow \sum_{j=1}^{n} p_j B_j \tag{1}$$

p_j and r_j are representing the stoichiometric coefficients of the product and reactant species. System gains equilibrium state on the equality of forward and backward reactions [2]. Therefore, for a reversible reaction, the law of mass action is valid.

$$R_s = R_s^+ - R_s^- \tag{2}$$

The molecular matrix identifies the balanced species of a reaction according to the rule of conservation of atoms (3).

$$Mx = Ct \tag{3}$$

The kinetic equation is represented by equation (4).

$$\frac{dx}{dt} = \Gamma R_x \tag{4}$$

The Lyapunov function for stability analysis is stated as (5):

$$G = \sum_{i=1}^{n} x_i \left[\ln\left(\frac{x_i}{x_i^{eq}} \right) - 1 \right] \tag{5}$$

Equation (5) uses the Lyapunov function G to illustrate the dissipative characteristics of bounded chemically reactive combinations, in accordance with the second law of thermodynamics. To reach an equilibrium state, the Lyapunov function (G) deviate from the equilibrium points during the transitional stage. Using the equilibrium point located on the initial approximation, each subsequent node can be evaluated by adding the shift vector (δx) given in equations (6) and (7) to the preceding node [9].

$$x_{n+1} = x_n + \delta x_n \tag{6}$$

$$\delta x_n = \sum_i v_i \rho_i \tag{7}$$

where ρ_i and v_i denote, respectively, the equation's null space basis. By establishing the shift vector's $\|\delta x_n\|$ for the grid's symmetrical configuration's structure in the absence of any constraints (8). By adjusting the parameters and $(q-1)$ independent vectors mi, geometric closure could be achieved and is represented by equation (9).

$$\sum \langle \tau_j, \rho_i \rangle v_i = -\left(\tau_j, \Delta G(x)\right) \tag{8}$$

$$\sum_{i=1}^{r} (m, \rho_i) v_i = \psi^2, \text{ where } \psi = 10^{-3} \tag{9}$$

The Jacobian Matrix L's eigenvalues is fundamental in developing the ILDM method.

$$\max\{Re[\lambda_i], i = 1, \cdots, (n-q)\} < h < \min\left\{ \begin{matrix} Re[\lambda_i], i = (n-q+1,) \\ \ldots n \end{matrix} \right\}, h < 0 \tag{10}$$

Using this method, the slow and fast eigenvalues of equation (10) are related in the fast subspace for every point that is transverse to the eigenvectors. The definition of the transition matrix (Q^*) is as follows:

$$Q^* = \left(v_1, \ldots, v_{n-q}, v_{n-q+1}, \ldots, v_n\right) \tag{11}$$

$v_1, \ldots, v_{n-q}$ are representing the fast eigenvectors of Jacobian matrix, and the slow one is represented by $v_{n-q+1}, \ldots, v_n$ (11). Let us consider the Q^{-1} (inverse matrix) in form of a row matrix:

$v_1, \ldots, v_{n-q}$ and $v_{n-q+1}, \ldots, v_n$ respectively, stand for the fast and slow eigenvectors of the Jacobian matrix. The Q^{-1} (inverse matrix) will be examined like a row matrix given in equation (12):

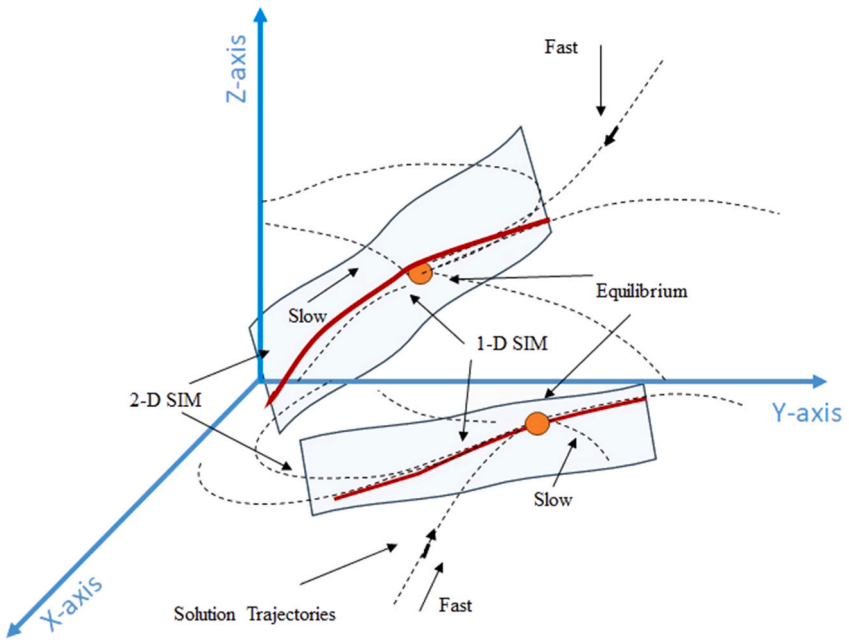

Fig. 1. Graphical representation of slow and fast solution trajectories and 1-D, 2-D slow invariant manifold in 3-D Phase Space.

$$Q^{-1} = \begin{pmatrix} v_1 \\ \cdots \\ v_{n-q} \\ v_{n-q+1} \\ \cdots \\ v_n \end{pmatrix} = \begin{pmatrix} Q_f^* \\ Q_s^* \end{pmatrix} \tag{12}$$

The ILDM equation by $(n-q)$ rows of Q_f^* is shadowed as (13):

$$Q_f^* . J \tag{13}$$

The ILDM method constructs a spectral projector using Schur decomposition. For further information on the ILDM approach, refer to Refs. [24,25].

2.2. The SIM

The SIM gives the low-dimensional route. In phase space, the solution trajectories of system migrate swiftly towards their lower-dimension and remain there till approaching the equilibrium slowly forms the basis for model reduction strategies.

To reduce the complex burden of reaction mechanism and to perform the geometrical investigation, the multi route complex chemical mechanism will be split down into different reaction routes by using the Horiuti rule see Fig. 1.

2.3. Sensitivity analysis (local)

The ILDM equation incorporates sensitivity analysis, a widely used concept in biochemical kinetic models and systems biology. Sensitivity analysis quantifies the influence of various variables on a species' response. This process involves applying local sensitivty analysis to examine the impact of variables of complex reactions. It also evaluates from equation (14) that how changes in output factors affect the input variables.

$$\overset{g}{x}_p = \frac{\partial x_i}{\partial t} = \lim_{\Delta\alpha_p \to 0} \frac{x_i(\alpha_p, \Delta\alpha_p) - x_i(\alpha_p)}{\Delta\alpha_p} \tag{14}$$

The ordinary differential system is displayed in equation (15).

$$\frac{dx_i}{dt} = R_i(X(t), Y(t)), i = 1, 2, 3, \ldots, m \tag{15}$$

The following is the Jacobian matrix presented in equation (16) for the sensitivity analysis using the system's chain law:

$$\delta = R_{k_p} + J.S, p = 1, 2, 3, \ldots, n \tag{16}$$

While R_{k_p} J and S are defined as in matrix form (17) as:

$$S = \begin{bmatrix} \frac{\partial x_1}{\partial \alpha_p} \\ \frac{\partial x_2}{\partial \alpha_p} \\ \cdots \\ \frac{\partial x_m}{\partial \alpha_p} \end{bmatrix}, H_{\alpha_p} = \begin{bmatrix} \frac{\partial R_1}{\partial \alpha_p} \\ \frac{\partial R_2}{\partial \alpha_p} \\ \cdots \\ \frac{\partial R_m}{\partial \alpha_p} \end{bmatrix}, J = \begin{bmatrix} \frac{\partial R_1}{\partial x_1} \cdots\cdots \frac{\partial R_1}{\partial x_1} \\ \frac{\partial R_2}{\partial x_1} \cdots\cdots \frac{\partial R_2}{\partial x_m} \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \frac{\partial R_m}{\partial x_1} \cdots\cdots \frac{\partial R_m}{\partial x_m} \end{bmatrix} \tag{17}$$

Thus, in the case of non-normalization, local sensitivity is determined as follows (18):

$$s_p^j = \frac{\partial x_j(t)}{\partial \alpha_p} \tag{18}$$

The local sensitivity is calculated using the half-normalization technique as follows 19):

$$s_p^j = \frac{1}{x(t)} \frac{\partial x_j(t)}{\partial \alpha_p} \tag{19}$$

Equation (20) presents the third technique, which is full normalization.

$$s_p^j = \frac{\alpha_p}{x(t)} \frac{\partial x_j(t)}{\partial \alpha_p} \tag{20}$$

Sensitivity analysis compares the impact of parameters using full, half and non-normalization techniques to identify the most sensitive parameter. Graphical results from these methods are analyzed to assess parameter sensitivity in different conditions.

3. Finding and discussions

Consider a three-step mechanism having seven chemical species to analyze the SQEM and ILDM. The reaction mechanism with its overall reaction step is given as under, graphically a three step mechanism is presented as in Fig. 2.

For convince let us consider the participating species as.

$c_1 = (Z_1), c_2 = (Z_2), c_3 = (AZ_1), c_4 = (BZ_2), c_5 = (A), c_6 = (B), c_7 = (AB)$. For verification of reaction routes, the Horiuti rule is applied to get the reaction routes. Although it is clear that the mechanism has only one reaction route and its Horiuti numbers are (1, 1, 1).

The stoichiometric matrix and their reaction rate equations are given as:

$$\left.\begin{matrix} r_1 \\ r_2 \\ r_3 \end{matrix}\right\} = \begin{bmatrix} -1.0 & 0.0 & 1.0 & 0.0 & -1.0 & 0.0 & 0.0 \\ 0.0 & -1.0 & 0.0 & 1.0 & 0.0 & -1.0 & 0.0 \\ 1.0 & 1.0 & -1.0 & -1.0 & 0.0 & 0.0 & 1.0 \end{bmatrix}$$

$$\begin{aligned} \mathrm{R_1(c)} &= \mathrm{k_1^+ c_1 c_2 \ - \ k_1^- c_3} \\ \mathrm{R_2(c)} &= \mathrm{k_2^+ c_2 c_6 \ - \ k_2^- c_4} \\ \mathrm{R_3(c)} &= \mathrm{k_3^+ c_3 c_4 \ - \ k_3^- c_1 c_2 c_7} \end{aligned} \tag{21}$$

The molecular matrix of above system (21) can be written in tabulated form as given in Table 1.

The initial parameters and rate constants are considered as arbitrary constants:

$$c_1^{eq} = .5, c_2^{eq} = .1, c_3^{eq} = .1, c_4^{eq} = .4, c_5^{eq} = .1, c_6^{eq} = .3, c_7^{eq} = .4$$

Where $\mathrm{k_1^+} = \frac{1}{2}, \mathrm{k_2^+} = 2, \mathrm{k_3^+} = \frac{12}{10}$A1

While the reverse reaction rate constants may be calculated by using the initial parameters and forward reaction rate constants. After calculating the rank of molecular matrix the key components of the system are three which is equal to the rank of molecular matrix. The system is now reduced into three chemical species according to their key components. $\dot{c_5}$, $\dot{c_6}$ and $\dot{c_7}$ (A, B and AB) by using Gibbs rule. The reduced form is as:

$$\begin{aligned} \dot{c_5} &= 0.15 \ - \ 0.25\mathrm{c_7} \ - \ (0.5\mathrm{c_5} + 0.5\mathrm{c_7})\big((\mathrm{c_6} + \mathrm{c_7} \ - \ 0.6) \ - \ 0.25\mathrm{c_5} \\ \dot{c_6} &= 0.165 \ - \ 0.15\mathrm{c_7} \ - \mathrm{c_6}(\mathrm{c_6} + 2\,\mathrm{c_7} \ - \ 1.2) \ - \ 0.05\mathrm{c_6} \\ \dot{c_7} &= (\mathrm{c_6} + \mathrm{c_7} \ - \ 1.1)(1.2\mathrm{c_5} + 1.2\mathrm{c_7} \ - \ 0.72) \ - \ \mathrm{c_7}(0.2\mathrm{c_5} + 2.4\,\mathrm{c_7})(\mathrm{c_6} + \mathrm{c_7} \ - \ 0.6) \end{aligned} \tag{22}$$

The microscopic solutions describes the examination of the key components particularly by following the particular transformation methods (22). This involves to study the least operational and functional modifications which takes place in the elements. The solution behavior of reduced key components are shown in Fig. 3.

The stability analysis is presented graphically in Fig. 4(a,b,c). This analysis provide a comprehensive visual representation of how each species responds to Variations and variations in system parameters.

In Table 2 specie AB is quickly converging to its equilibrium point as compared with A and B. This reflection emphasizes the stability and equilibrium properties of the system, demonstrating the consistency and dependability of the reaction model in seizing the dynamic behavior of the chemical process. These findings highlight the importance of understanding the transitional dynamics of

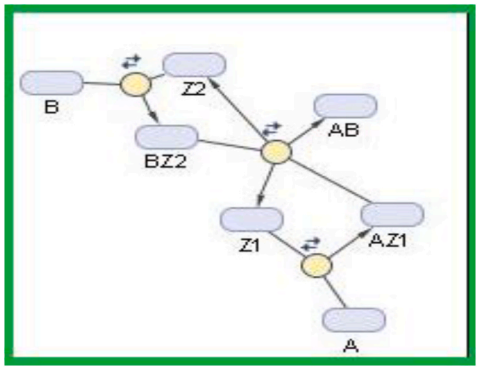

Fig. 2. Graphical behavior of multi-step mechanism.

Table 1
The molecular martix.

	Z_1	Z_2	A	AZ_1	BZ_2	B	AB
Z_1	1.0	0.0	0.0	1.0	0.0	0.0	0.0
Z_2	0.0	1.0	0.0	0.0	1.0	0.0	0.0
A	0.0	0.0	1.0	1.0	0.0	0.0	1.0
B	0.0	0.0	0.0	0.0	1.0	1.0	1.0

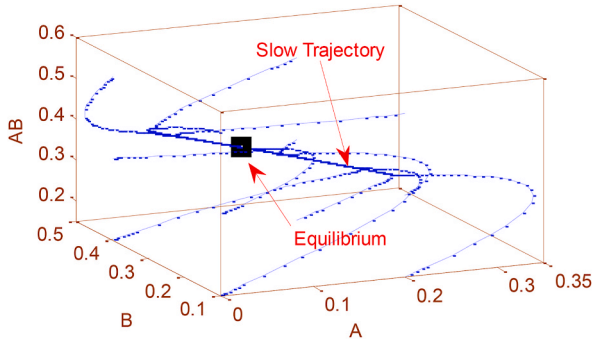

Fig. 3. Solution trajectories (microscopic solutions) of reduced species A, B and AB.

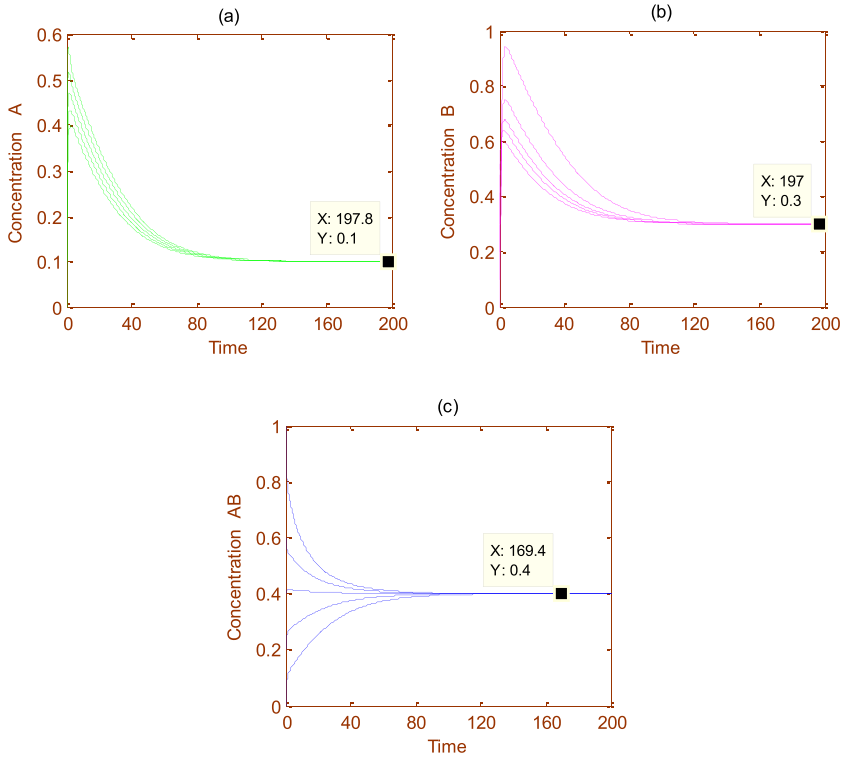

Fig. 4. Steady-state behavior of reduced chemical species A, B and AB approaching towards their equilibrium point after completing their transition time period.

the key components, thereby elucidating their role in main the scheme's overall behavior.

The analysis of one dimensional manifolds are aided in the current investigation using SQEM and the ILDM for elements A,B, and AB. The mathematical results obtained have been plotted to effectively replicate a SIM. In the SQEM technique the approximate solution is obtained by choosing the slowest left eigen vector obtained through Jacobian matrix (at equilibrium state). In Fig. 5(a) approximation curve is shown and in 5(b) along trajectories. Dividing the phase-space into fast/slow phase-spaces by slowest eigen

Table 2
Time period of chemical species approaching toward their equilibrium point.

Species	A	B	AB
Time span	197.80	197.00	169.40
Eq. point	0.1	0.3	0.4

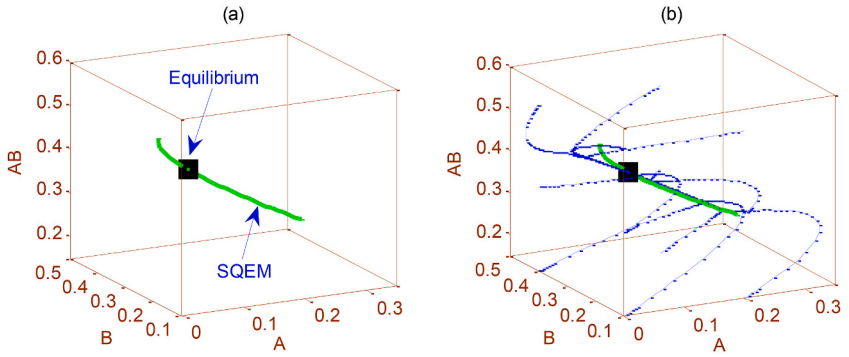

Fig. 5. Approximate solution obtained through SQEM and approximated solution curve along with solution curves given in (a) and (b) respectively.

vectors evaluation. Each next node of approximated curve with a standard step-size of the overall route is graphically presented in Fig. 6 (a) and in 6(b) along trajectories. For overall route, the comparison between SQEM and ILDM is examined in Fig. 7 (a) and in 7(b) along solution trajectories. Notably, the investigation demonstrated that the results obtained using the ILDM are more precise than those obtained using the SQEM. When compared to the ILDM results, the SQEM results clearly show more significant change from invariant region. These results highlight the essential significance that computational technique selection plays in effectively capturing the fundamental dynamics of the chemical system.

3.1. Sensitivity analysis

The augmentation of three sensitivity analysis normalization procedures are used to show how input factors affect output variables in a system. These different techniques to check the sensitivity analysis of the system are non, half and full-normalization. The results of these techniques can be seen in the graph below. The assessment of the first method, which utilizes non-normalization, is presented in Fig. 8(a), which demonstrates that the species A is more sensitive in reaction 1 with respect to k_1^- (backward rate of constant). Fig. 8(b), which demonstrates the half-normalization strategy, shows that the species AZ is more sensitive with respect to K_1^- direction. As shown in Fig. 8(c), the graph indicates full normalization technique that shows the species BZ displays more sensitive in both the K_1^+ and K_1^- directions.

4. Comparison

Researchers have used numerous model reduction strategies on a variety of chemical reaction processes. The three reduction techniques QEM, SQEM, and ILDM are the main topics of this research study. Using both graphical and tabular representations, we systematically assess and compare the efficacy and correctness of the solution curves derived using various methodologies. We want to

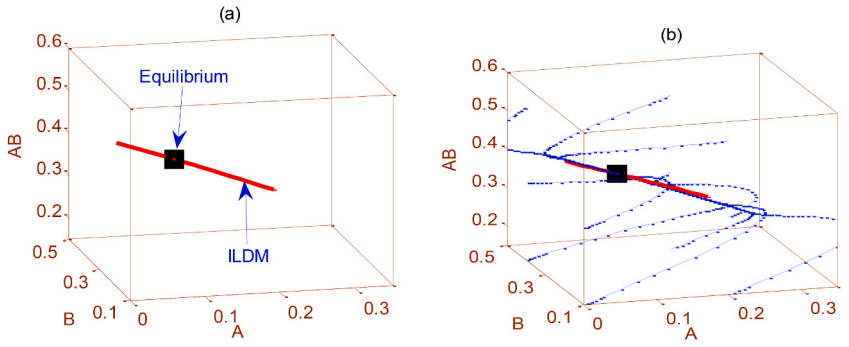

Fig. 6. Approximate solution obtained through ILDM and approximated solution curve along with solution curves given in (a) and (b) respectively.

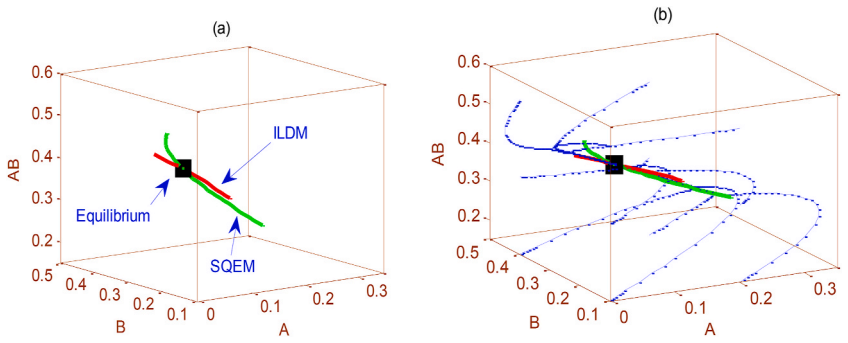

Fig. 7. Comparison between SQEM and ILDM curves.

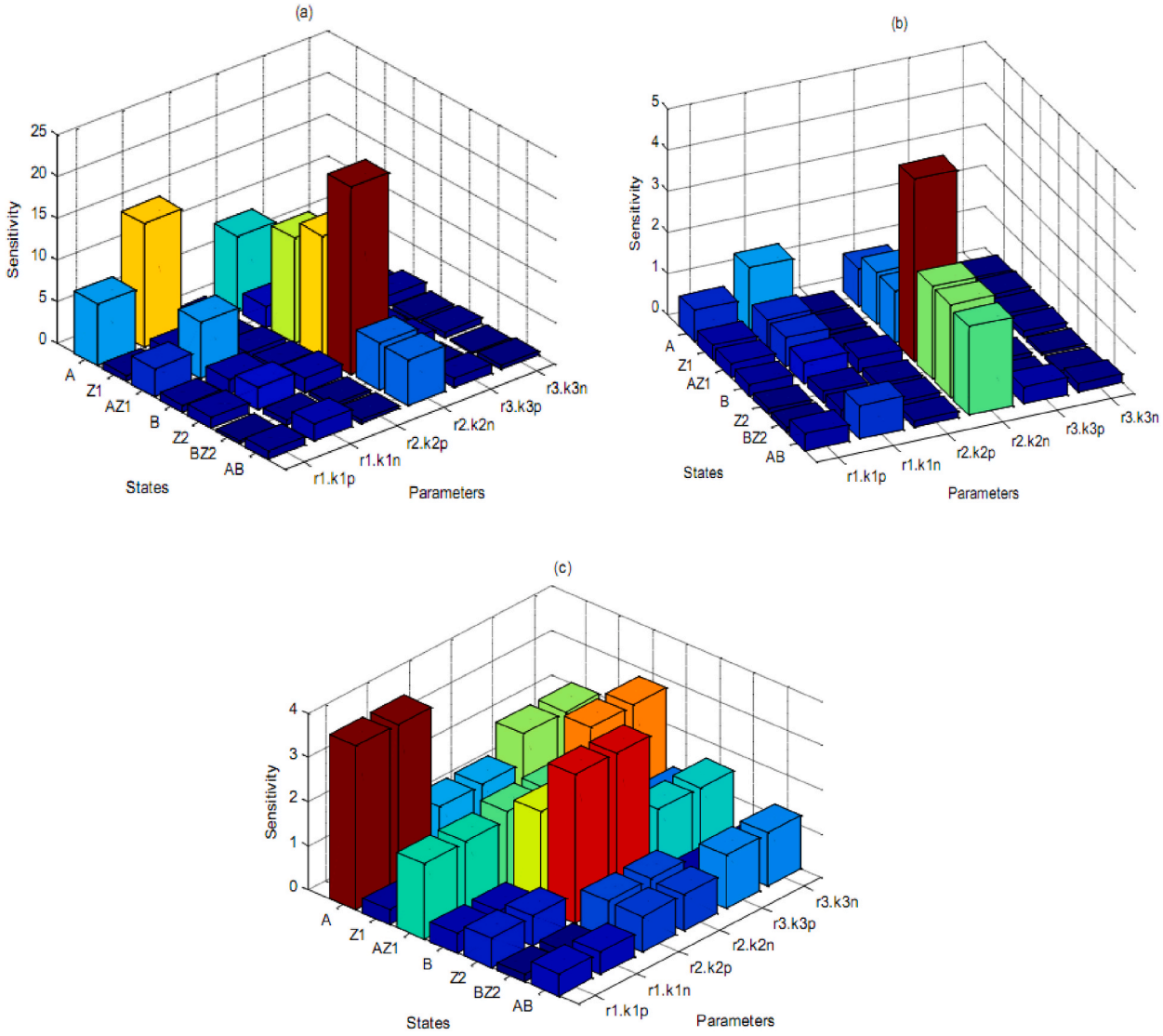

Fig. 8. The consequences of a local sensitivity analysis for all species inside the complex system employing (a) no normalization, (b) half-normalization approach and (c) complete normalization approach.

Table 3
Shows the difference between SQEM and ILDM for some points.

Sr. No	SQEM result			ILDM result			Absolute Differences		
	A	B	AB	A	B	AB	A	B	AB
1	0.1501	0.3481	0.3538	0.1573	0.3370	0.3576	0.0070	0.0031	0.0048
2	0.1365	0.3587	0.3654	0.1433	0.3279	0.3685	0.0058	0.0028	0.0041
3	0.1238	0.3292	0.3771	0.1293	0.3189	0.3794	0.0045	0.0023	0.0033
4	0.1153	0.3197	0.3890	0.1152	0.3099	0.3802	0.0029	0.0018	0.0022
5	0.1000	0.3000	0.4000	0.1000	0.3000	0.4000	0.0000	0.0001	0.0000
6	0.0877	0.2903	0.4120	0.0857	0.2912	0.4108	0.0020	0.0009	0.0012
7	0.0758	0.2805	0.4243	0.0713	0.2824	0.4216	0.0045	0.0019	0.0027
8	0.0642	0.2705	0.4367	0.0568	0.2737	0.4323	0.0074	0.0032	0.0044
9	0.0531	0.2604	0.4492	0.0423	0.2651	0.4431	0.0108	0.0047	0.0061
10	0.0425	0.2501	0.4619	0.0276	0.2566	0.4538	0.0149	0.0065	0.0081

evaluate each strategy's efficacy and validity in producing solution curves using this study given in Table 3.

5. Conclusion

The implementation of the modern model reduction approaches is useful to get around the rigidity and complexity of reaction processes. Even when states and steps are well specified, the presence of several distinct states and steps inside a system not only makes it more complicated but also makes it difficult to compare different states and steps. Therefore, the overview of established reduction strategies for chemical kinetics modelling in complicated systems is presented in this article. To gain a deeper understanding of the refined dynamics within intricate chemical processes, our focus lies on assessing the stability of the model at chemical equilibrium points. A depth examination of the steady-state approximation helps us understand how chemical reactions develop over time and eventually reach a balanced state. Sensitivity analysis reveals how changes in input parameters impact species behavior in complex systems, identifying key variables crucial for optimizing and managing chemical processes. According to our results comparison the curve form by SQEM and ILDM, it is observed that ILDM solution is more accurate than SQEM. According to our results, the curves generated by the ILDM and SQEM which method is more accurate than SQEM method.

CRediT authorship contribution statement

Xiao Xin: Writing – review & editing, Visualization, Formal analysis. **Faisal Sultan:** Supervision, Methodology, Investigation, Conceptualization. **Muhammad Yaseen:** Methodology, Formal analysis. **El-Sayed M. Sherif:** Writing – review & editing, Visualization, Validation, Formal analysis. **Muhammad Shoaib Ishaq:** Software, Investigation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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