Spatio-Temporal Chaos in Belousov – Zhabotinsky Systems Modelling & Experimental Characterization

Author: Sarthak Singh, Department of Chemical Engineering, IIT Kanpur
Mentor: Prof. Dipin S. Pillai, Department of Chemical Engineering, IIT Kanpur

INTRODUCTION

The **Belousov–Zhabotinsky (BZ) reaction** is a foundational example of a nonlinear, non-equilibrium chemical oscillations that form fascinating spatio-temporal patterns such as target and spiral waves. Mathematically, the reaction is often modeled using the Field–Körös–Noyes (FKN) mechanism and its simplified version, the **Oregonator**, which captures the core dynamics in a manageable framework.

In this study, we work with the **Oregonator model** to simulate the temporal and spatial oscillations observed experimentally, and compare the model outputs with RGB-extracted data from recorded BZ reactions. This approach allows us to quantify the accuracy of the model and explore its capability to reproduce real-world chemical patterns.

EXPERIMENTAL METHODS

The experimental protocol for the BZ reaction was adapted from Arthur T. Winfree's **"The Geometry of Biological Time"**, which outlines a reliable approach for observing temporal oscillations and spatio-temporal wave patterns.

Four separate solutions were prepared:

- **Solution A**: 2.57 g $NaBrO_3$ + 34.57 mL H_2O + 1.08 mL H_2SO_4 (99%)
- **Solution B**: 1 g Malonic Acid in 10 mL H_2O (used 6 mL)
- **Solution C**: 1 g NaBr in 10 mL H_2O (used 3 mL)
- **Solution D**: Ferroin indicator solution (used 6 mL)

Figure 1: Shows a beaker containing **deep red solution** (formed after mixing all the solutions)

Protocol:

1. In a beaker, combined 6 mL of **Solution A** and 6 mL of **Solution B**.
2. Added 3 mL of **Solution C** to the mixture.
3. Finally, added 6 mL of **Solution D** to initiate the redox oscillations.
4. Observed color changes (red ↔ blue) in the beaker for 5–10 oscillation cycles.
5. Transferred the solution into a shallow **Petri dish** (~10 cm diameter) to visualize wave propagation.
6. Recorded the reaction from above to capture both **temporal oscillations** and **target wave patterns**.

Figure 2: Shows the same beaker after the solution is turned **blue**, in color illustrating the characteristic color change of BZ reaction.

RESULTS

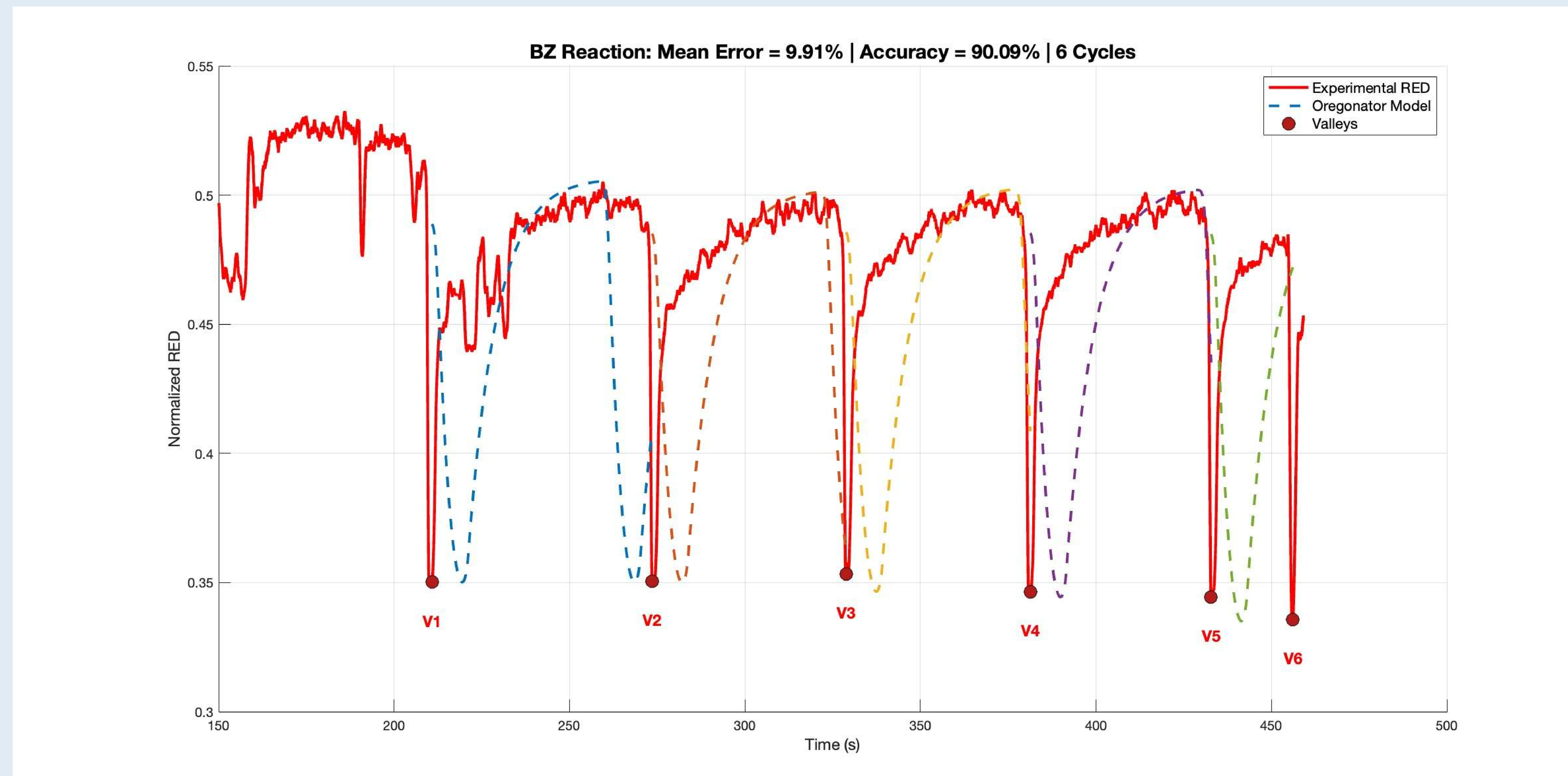


Figure 3: The solid red line shows the experimentally measured normalized RED (Relative Extinction Difference) over time, while the dashed lines represent the Oregonator model's predictions for each cycle. The close alignment between the two indicates that the model effectively captures the system's oscillatory behavior. The labeled points (V1–V6) mark the valleys, or minima, in each oscillation cycle. These valleys are critical for analyzing the periodicity and stability of the reaction.

Figure 4: The petri dish shows the initial stage of colony growth, with subtle swirling patterns beginning to form along the edges.

Figure 5: The colony patterns become more pronounced, with larger, distinct circular formations emerging across the surface.

Figure 6: The swirling concentric ring patterns are developed, covering much of the dish displaying increased complexity.

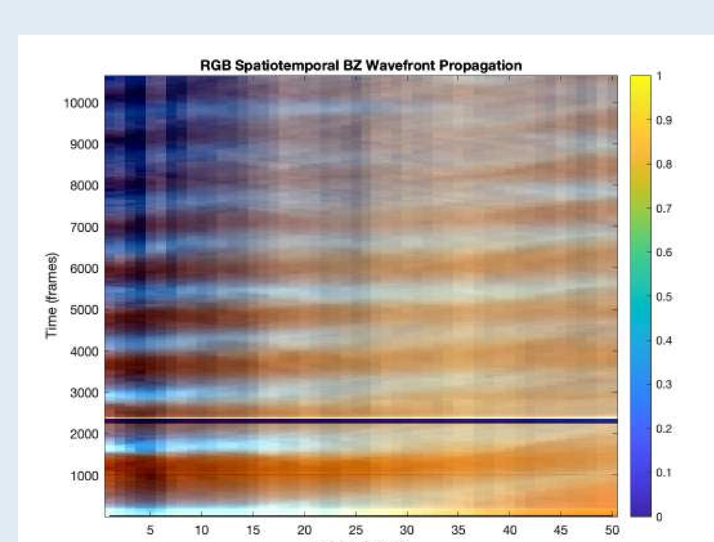


Figure 7: This plot displays the spatiotemporal evolution of color intensity in the BZ reaction, with the color bar on the right indicating normalized values from low (blue) to high (yellow) across radius and time.

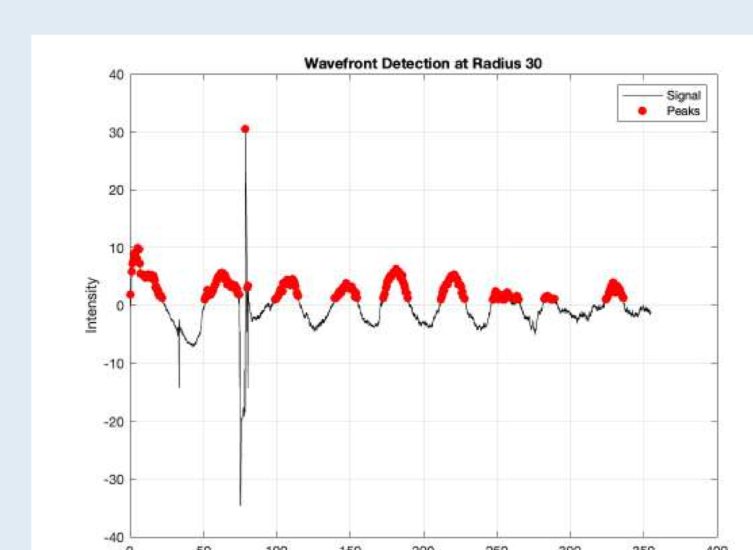
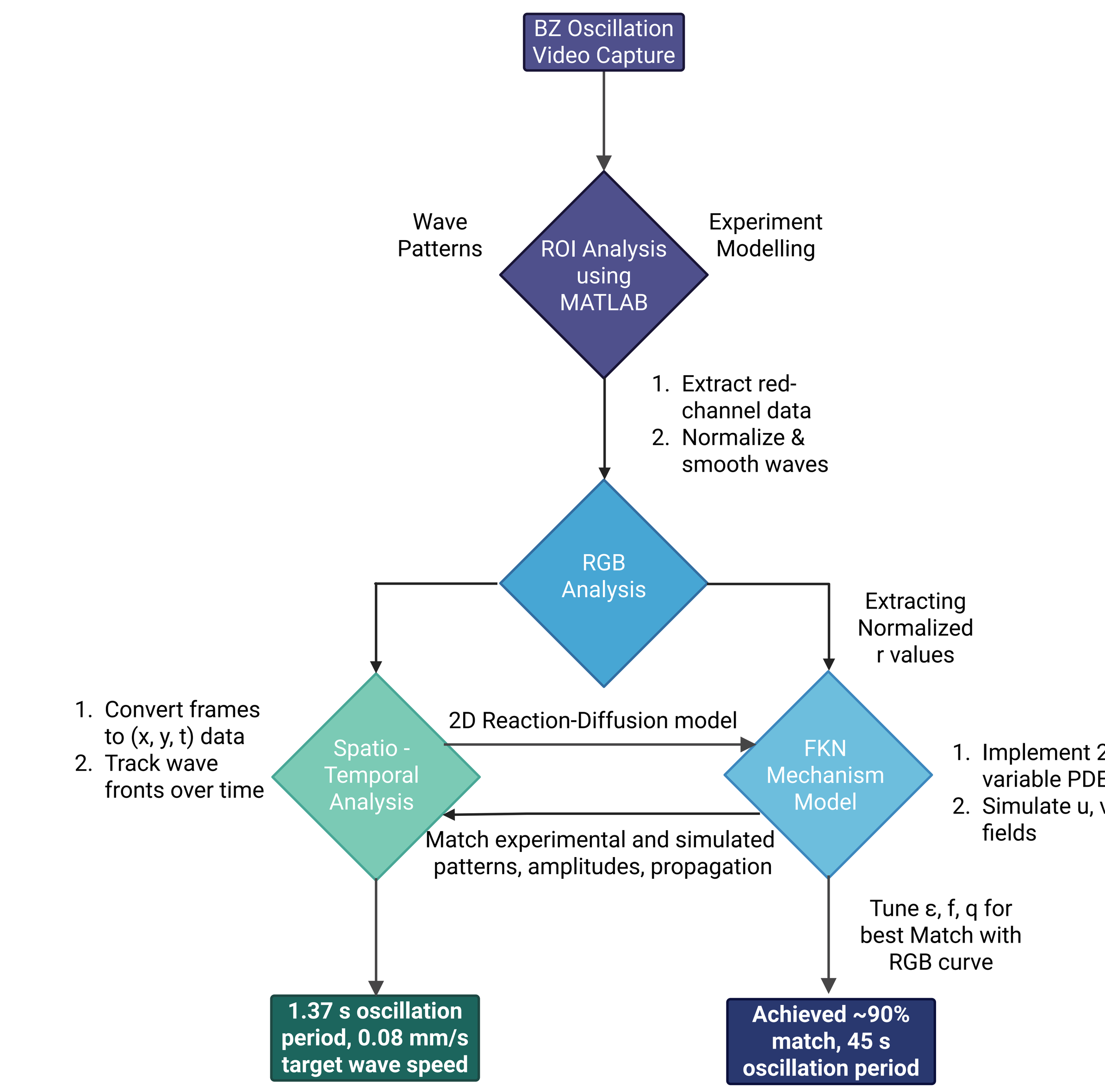


Figure 8: This curve displays the intensity of chemical wavefronts detected at a fixed radius over time, highlighting the periodic peaks that correspond to the arrival of successive target waves in the Belousov-Zhabotinsky reaction.

SIMULATION WORK OVERFLOW



OBSERVATIONS & FUTURE SCOPE

- Periodic color oscillations were observed due to the ferroin indicator, with cycles averaging ~**45 seconds**.
- Among RGB channels, the **red** channel exhibited the most distinct contrast, making it optimal for tracking oscillations.
- A strong correlation with accuracy of **~90%** was established between the red channel's normalized intensity plot and the Oregonator model.
- Final parameter estimates from the model: $\varepsilon=0.05, f=1.4, q=0.002$
- The BZ reaction generated well-defined concentric (target) waves, with the first wave typically appearing **3–5 minutes** after initiation.
- Wavefront propagation speed, extracted from spatiotemporal RGB intensity profiles, averaged **0.08 mm/s**, aligning well with published values.
- Wavefront distortion due to vibrations or airflow emphasized the importance of maintaining a stable and undisturbed setup.

In future, we would work on transition to experiments in gel media to observe more stable and structured wave dynamics in quasi-2D and 3D systems. Explore alternate model **Brusselator** for capturing a wider range of pattern behaviors, including reaction-diffusion instabilities in gels, and study chaos.

REFERENCES

1. An Analysis of the Belousov-Zhabotinskii Reaction An Analysis of the Belousov-Zhabotinskii Reaction (Casey Gray)
2. Study on the Formation of Complex Chemical Waveforms by Different Computational Methods (Jiali Ai, Chi Zhai, Wei Sun)
3. ArthurT.Winfree's The Geometry of Biological Time (Chapter 11)