

# Spatial and temporal dynamics of Belousov-Zhabotinsky reaction: A STEM approach

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An integrative methodology for teaching science is proposed through the STEM methodology (Science-Technology-Engineering-Mathematics). The STEM methodology provides students the opportunity to combine knowledge in an interdisciplinary and collaborative manner, allowing the development of creative and systemic thinking. As a model, we propose the experimental reproduction of the Belousov-Zhabotinsky reaction (BZ), which is the standard prototype of nonlinear chemistry. Besides, we used the Python V2.7 programming software and the Jupyter platform for the computational reproduction of the BZ reaction. The STEM methodology could help the development of new competences for students; that is, it will provide them with tools to solve complex current problems that require the interdisciplinarity.

**Keywords:** STEM methodology; teaching; multidiscipline; Belousov-Zhabotinsky reaction (BZ); nonlinear chemistry; python V2.7; reaction-diffusion system.

Se propone una metodología integradora para la enseñanza de la ciencia a través de la metodología STEM (Ciencia-Tecnología-Ingeniería-Matemáticas), por sus siglas en inglés. La metodología STEM brinda a los estudiantes la oportunidad de combinar el conocimiento de manera interdisciplinaria y colaborativa, lo que favorece el desarrollo del pensamiento creativo y sistémico. Como modelo, se sugiere la reproducción experimental de la reacción Belousov-Zhabotinsky (BZ), que es el prototipo estándar de la química no lineal. Además, se utilizan el lenguaje de programación Python V2.7 y la plataforma Jupyter para la reproducción computacional de la reacción BZ. La metodología STEM podría ayudar al desarrollo de nuevas competencias para los estudiantes; es decir, les proporcionará herramientas para resolver problemas actuales complejos que requieren de la interdisciplinariedad.

**Descriptores:** Metodología STEM; enseñanza; multidisciplinaria; reacción Belousov-Zhabotinsky (BZ); química no lineal; python V2.7; sistemas de reacción-difusión.

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## 1. Introduction

STEM studies (Science-Technology-Engineering-Mathematics) are of great importance for the economic development of any country [7]. Martini *et al.*, propose that it is necessary to implement the STEM methodology to create a *Maker* culture in the population, that is, a community that is highly resilient and that seeks solutions to real problems with a holistic approach and through integrative tools. However, to achieve this, teachers must be able to establish *Makerspaces*

[27]. On the other hand, Dómeneche proposes project-based learning as a strategy to implement STEM studies and also describes the incorporation of arts and humanities to provide *creativity* to STEAM studies (Science-Technology-Engineering-Arts-Mathematics). The implementation of the arts and humanities, seeks that individuals develop the *soft – skills*, which is related to the ability to relate to other individuals, collaborative work, communication skills, etc [11]. When implementing STEAM studies, it is sought that individuals, in addition to possessing or developing scientific



## 1.2. Python programming language

Python is a programming language suitable for both scientific computing and teaching, and it is a programming language that can be used with multiple interpreters or development environments. Here are the most commonly used Python distributions:

- Anaconda: [www.anaconda.org/anaconda/python](http://www.anaconda.org/anaconda/python)
- Enthought Canopy: [www.enthought.com](http://www.enthought.com)
- PyCharm: [www.jetbrains.com/pycharm/](http://www.jetbrains.com/pycharm/)

Python is a multi-paradigm programming language, which, thanks to its wide variety of packages, can be used for multiple tasks. It has libraries and modules for various applications ranging from numerical calculation (Numpy: [www.numpy.org/](http://www.numpy.org/)), scientific computing (Scipy: [www.scipy.org](http://www.scipy.org)), analysis and data processing (Pandas: [www.pandas.pydata.org](http://www.pandas.pydata.org)), Machine Learning (scikitlearn: [www.scikit-learn.org](http://www.scikit-learn.org)), as well as for specific areas such as chemical engineering (Cantera: [www.cantera.org](http://www.cantera.org)). Python is free software (freeware) and exists for all operating systems and can be easily linked with other programming languages such as C ([www.cython.org/](http://www.cython.org/)), Fortran ([www.fortranwiki.org/fortran/show/Python](http://www.fortranwiki.org/fortran/show/Python)), Java (<http://www.jython.org/>), R ([www.rpy2.bitbucket.io/](http://www.rpy2.bitbucket.io/)), and specialized software such as Matlab ([www.pypi.python.org/pypi/pymatbridge](http://www.pypi.python.org/pypi/pymatbridge)). Next, we write the code in Python of the program that simply shows the word "Hello World"; in Python, it is written as simple as:

```
In [ ]: print('Hello_World')
```

As well as the graph of mathematical functions:

```
In [ ]: import numpy as np
import matplotlib.pyplot as plt
X=[]
Y=[]
for x in np.arange(0,100,10):
    y=x**2
    X.append(x)
    Y.append(y)
plt.plot(X,Y,'rp')
```

or, written in another form:

```
In [ ]: import numpy as np
import matplotlib.pyplot as plt

x=np.linspace(0,100,10)
plt.plot(x,x**2,'rp')
plt.show()
```

Python is a versatile programming language. Therefore, in this paper, we propose to this programming language as a fundamental tool for learning STEM.

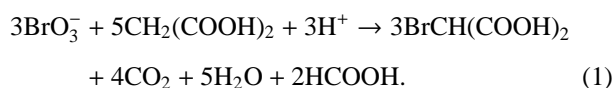
## 2. Methodology

The methodology is divided into three sections, the first of which consists of the mathematical description of the BZ reaction. A system of nonlinear differential equations is proposed to describe the dynamics underlying the BZ reaction. The second section describes the computational methodology for the numerical solution of the model proposed in Sec. 2.1. Finally, the third section consists the experimental reproduction of the BZ reaction. The student, with the help of the teacher, must correlate the results obtained from the proposed methodologies, with the aim of the student building knowledge with a systemic approach.

### 2.1. Theoretical Methodology

The kinetic scheme originally proposed by Field, Körös, and Noyes (FKN) is the most common chemical mechanism to describe the dynamics of the BZ reaction [13]. Nevertheless, it is not the only one, there are different chemical models that try to explain the dynamics of the reaction BZ considered that intermediate chemical species, such as MA\* or Br\* would play an important role in the feedback mechanism of the reaction, such is the case of the Radicalator [22,18,29]. However, the FKN model has proved so robust that it is possible to reduce it to a much simpler model called Oregonator [41,13]. To obtain all these mathematical models, it is possible to use the standard techniques of chemical kinetics [28].

The overall chemical equation of the BZ reaction is as follows [19]:



After several years of research, the BZ reaction mechanism could be elucidated, encountering a mechanism consisting of 27 chemical species and a total of 80 chemical reactions [22,19].

The Oregonator can be obtained from a very simple reaction mechanism composed essentially of five irreversible steps [41]. By the following change of variable,  $A = \text{BrO}_3^-$ ;  $B =$  organic species such as malonic acid and bromo malonic acid;  $P = \text{HOBr}$ ;  $X = \text{HBrO}_2$ ;  $Y = \text{Br}^-$ ;  $Z =$  the oxidized form of the catalyst;  $f$  is a stoichiometric coefficient [41]:



Whose laws of reaction rate are [41]:

$$v_2 = k_2[A][Y] \quad (7)$$

$$v_3 = k_3[X][Y] \quad (8)$$

$$v_4 = k_4[A][X] \quad (9)$$

$$v_5 = k_5[X]^2 \quad (10)$$

$$v_6 = k_6[B][Z]. \quad (11)$$

To construct the Oregonator model, it is necessary to assume that the concentrations of  $A$  and  $B$  remain constant (they are associated with the initial concentrations of the precursors). Subsequently, it has to apply the standard techniques of chemical kinetics to obtain the dynamic model considering  $X$ ,  $Y$ , and  $Z$  as dynamic variables, assuming that chemical reactions are elementary, that is, stoichiometric coefficients coincide with the power of dynamic variables [41,28]. The speed laws for Eqs. (2) - (6) are shown in Eqs. (7) - (11). The equations of speed for the variables  $X$ ,  $Y$ , and  $Z$  are:

$$\frac{d[X]}{d\tau} = k_2[A][Y] - k_3[X][Y] + k_4[A][X] - 2k_5[X]^2, \quad (12)$$

$$\frac{d[Y]}{d\tau} = -k_2[A][Y] - k_3[X][Y] + 1/2fk_6[B][Z], \quad (13)$$

$$\frac{d[Z]}{d\tau} = 2k_4[A][X] - k_6[B][Z]. \quad (14)$$

Where the  $k_i$  corresponds to the reaction rate constants and  $\tau$  is the time. The analysis is simplified by converting these equations into a dimensionless form [41]. Using the following variable changes:

$$x \equiv \frac{2k_5[X]}{k_4[A]}, \quad y \equiv \frac{k_3[Y]}{k_4[A]},$$

$$z \equiv \frac{k_c k_5[B][Z]}{(k_4[A])^2}, \quad t \equiv k_c[B]\tau.$$

Multiplying both sides of Eq. (12) by  $(2k_5/k_4[A])$

$$\frac{2k_5}{k_4} \frac{dx}{d\tau} = (k_2[A][Y] - k_3[X][Y] + k_4[A][X] - 2k_5[X]^2) \frac{2k_5}{k_4[A]}$$

distributing terms,

$$= \frac{2k_2k_5}{k_4} [A][Y] - \frac{2k_3k_5}{k_4[A]} [X][Y] + \frac{2k_4k_5}{k_4[A]} [A][X] - \frac{2k_5^2}{k_4[A]} [X]^2$$

factorizing  $k_4[A]$ ,

$$= k_4[A] \frac{2k_2k_5}{k_4} [A][Y] - k_4[A] \frac{2k_3k_5}{k_4[A]} [X][Y] + k_4[A] \frac{2k_4k_5}{k_4[A]} [A][X] - k_4[A] \frac{2k_5^2}{k_4[A]} [X]^2$$

Realizing the change of variable for  $x$ ,  $y$ , and  $t$ ,

$$\frac{k_6[B]}{k_4[A]} \frac{dx}{dt} = qy - xy + x - x^2.$$

It is renamed:

$$\frac{k_6[B]}{k_4[A]} \equiv \varepsilon.$$

By performing the same procedure for the variables  $y$  and  $z$  the following system of nonlinear differential equations is obtained [41]:

$$\frac{dx}{dt} = \frac{qy - xy + x(1-x)}{\varepsilon} \quad (15)$$

$$\frac{dy}{dt} = \frac{-qy - xy + fz}{\varepsilon'} \quad (16)$$

$$\frac{dz}{dt} = x - z, \quad (17)$$

where  $\varepsilon' \equiv (2k_5k_6[B])/k_3k_4[A]$  and  $q \equiv (2k_5k_2/k_3k_4)$ . The typical values of the parameters are:  $\varepsilon \approx 10^{-2}$ ,  $\varepsilon' \approx 10^{-5}$ ,  $q \approx 10^{-4}$ , and  $t$  it is dimensionless time. As the parameter  $\varepsilon' \approx 10^{-5}$ , it is possible to consider the approximation of the steady-state of the variable  $y$ , therefore,  $y \equiv (fz/q + x)$  then the Eqs. (15) - (17) are reduced to [41]:

$$\varepsilon \frac{dx}{dt} = x(1-x) + f \frac{q-x}{q+x} z \quad (18)$$

$$\frac{dz}{dt} = x - z \quad (19)$$

In this way, the Oregonator model shows the typical form of a chemical feedback system, that is, the variable  $x$  functions as an activator, while the variable  $z$  has the role of the inhibitor [41]. This model is so robust that it describes the phenomenology of the BZ reaction. The Eqs. (18) - (19) correspond to a system of dimensionless nonlinear differential equations. If to the Eqs. (20) - (21) terms associated with diffusion are added, the system becomes:

$$\varepsilon \frac{dx}{dt} = x(1-x) + f \frac{q-x}{q+x} z + D_x \nabla^2 x \quad (20)$$

$$\frac{dz}{dt} = x - z + D_z \nabla^2 z, \quad (21)$$

where  $D_x$  and  $D_z$  are the dimensionless diffusion coefficients, and  $\nabla^2$  is the Laplacian operator (see Appendix A). To solve the system of Eqs. (18) - (19) and the system of Eqs. (20) - (21), it is necessary to implement numerical methods and computational simulation tools.

## 2.2. Computational Methodology

For the numerical solution of the Eqs. (18) - (19), the Euler numerical method was used with the following values of the parameters:  $\varepsilon \equiv 0.03$ ,  $q \equiv 0.015$  and  $f \equiv 1.0$ , with a step of time  $dt \equiv 0.0001$ . The numerical values of the parameters were selected according to the linear stability criteria for the Eqs. (18) - (19). With these parameter values, the system shows periodic oscillations, which correspond to a limit cycle [34]. The code in Python would be:

```
In [ ]: #Import modules
import numpy as np
#Module for arrays
import matplotlib.pyplot as plt
#Module for graphics

#Model parameters
f=1.0
q=0.015
e=0.03

#Numerical method parameters

t0=0.0 #Initial time
tf=100.0 #Final time
dt=0.0001 #Time step

#Initial Condition
X0=0.5
Z0=0.5

#Functions
def fun1(x,z):
    return (x*(1-x)
            +f*z*((q-x)/(q+x)))/e
def fun2(x,z):
    return x-z

#Lists for data
X=[] #List for x variable
Z=[] #List for z variable
T=[] #List for time values

#Assign initial condition
x=X0
z=Z0

#Numerical method
for t in np.arange(t0,tf,dt):
    t=t+dt
    #Euler rule for x variable
    x=fun1(x,z)*dt+x
    # Euler rule for z variable
    z=fun2(x,z)*dt+z
    X.append(x) #List for x variable
    Z.append(z) #List for z variable
    T.append(t) #List for t variable

#Plot construction
f, axes= plt.subplots(1,2,
figsize=(14,6))
axes[0].plot(T,X,'b.',label='x')
axes[0].plot(T,Z,'k',label='z')
axes[0].set_title('Oscillations',
size=16)
axes[0].set_xlabel('t [adimensional]',
size=14)
axes[0].set_ylabel('x,z [adimensional]',
size=14)
axes[0].legend(loc='best')
axes[1].plot(X,Z,'g*', label='Phase Space')
```

```
axes[1].set_title('Phase Space', size=16)
axes[1].set_xlabel('x [adimensional]',
size=14)
axes[1].set_ylabel('z [adimensional]',
size=14)
axes[1].legend(loc='best')

plt.show()
```

For the numerical solution of the Eqs. (20) - (21), the numerical method of discretization by finite differences was used, under the condition of Neumann contour. The following values of the parameters were used:  $\varepsilon \equiv 0.03$ ,  $q \equiv 0.015$ ,  $f \equiv 2.0$ , with a time step  $dt \equiv 0.001$ , a spatial step  $dh \equiv 0.5$ ,  $D_x \equiv 2.0$  and  $D_z \equiv 0.0$ . The code used to numerically integrate the Eqs. (20) - (21) is described below.

```
In [ ]: from Larray import*
#Reaction-Diffusion module
from Lgraphicarray import *
#Complement of Larray
#Model Parameters
e=0.03
q=0.015
f=1.0
Dx=2.0
N=2.5*(1.e-4)

#Space-temporal parameters
l=256
L=(1,1)
count=0
DISPLAY=100
t0=0.0 #Initial Time
tf=10000.0 #Final Time
dt=0.001 #Time Step
dh=0.5 #Space step

#Functions
def fun1(x, z):
    s = (x/e)*(1-x)-
        ((f*z)/e)*((x-q)/(x+q))
    return s

def fun2(x, z):
    s = x-z
    return s

#Laplace Operator
def F(U):
    return array([ fun1(U[0], U[1]) ,
fun2(U[0], U[1])])

def Lap(U):
    return array([ Dx*Lap_9(U[0],dh)
, zeros(L)])
```

```

#Initial condition
x0 = 0.5
z0 = 0.5
A = x0*ones(L)
I = z0*ones(L)
A[1/2-5:1/2+5, 1/2-5:1/2+5]=1.0-x0
U = array([A,I])

#Making canvas
G = GraphicArray(L,
RGB=["ffff6", "", "ee5611"])
G.set_title('BZ Reaction')
G.display(U[0])

#Numerical method
t=0
while t < tf:
    t = t + dt
    if count % DISPLAY == 0:
        G.display(U[0])
        G.time(t)
    #Euler rule
    U = U + ( F(U) + Lap(U) )*dt
    #Frontier conditions
    setFrontierZeroDeriv(U[0])
    seed()
    if random((1)) < N :
        si=randint(1,45,(1))[0]
        sj=randint(1,45,(1))[0]
        sec=(1.0-x0)*ones((si,sj))
        i=randint(0,99-si,(1))[0]
        j=randint(0,99-sj,(1))[0]
        U[0][i:i+si,j:j+sj]=sec
    count += 1

```

### 2.3. Experimental Methodology

The following solutions were prepared for the experimental reproduction of the BZ reaction:

A: 5 g of  $\text{KBrO}_3$  (potassium bromate) (Sigma-Aldrich) in 67 mL of deionized water ( $\rho \cong 18.2 \text{ M}\Omega\text{cm}$ ) was added. (Concentration: 0.45 M). This solution was prepared at  $30^\circ\text{C}$  and constant stirring for 5 min to increase the solubility of  $\text{KBrO}_3$ . Subsequently, it was allowed to cool to room temperature.

B: 1 g of  $\text{KBr}$  (potassium bromide) (Sigma-Aldrich) in 10 mL of deionized water ( $\rho \cong 18.2 \text{ M}\Omega\text{cm}$ ) was added. (Concentration: 0.84 M).

C: 1 g of  $\text{C}_3\text{H}_4\text{O}_4$  (malonic acid) (Sigma-Aldrich) in 10 mL of deionized water ( $\rho \cong 18.2 \text{ M}\Omega\text{cm}$ ) was added. (Concentration: 0.96 M).

Once the solutions were prepared, 12 mL of solution A, 1 mL of solution B, 2 mL of solution C and 1 mL of  $\text{H}_2\text{SO}_4$  (sulfuric acid) (Sigma-Aldrich (96 %)) were added to a beaker. At this point, the mixture acquires a yellow hue due to the presence and release of  $\text{Br}_2$  (molecular bromine),

so that the solution is kept under constant stirring with the help of a magnetic stirrer and an electric grill until the said mixture acquires a hue transparent. Finally, 1 mL of  $[\text{Fe}(\text{o-phen})_3]\text{SO}_4$  (ferroin)(Sigma-Aldrich) was added as an indicator for the chemical reaction to visualize the color changes. Once the chemical reaction started, 3 mL of the mixture was extracted from the beaker and placed in a watch glass without stirring to observe the formation of temporal space patterns.

### 3. Results and comments

In Fig. 2, we can see the experimental reproduction of the BZ reaction. The duration time of the oscillations in the BZ reaction (using the experimental procedure described in the experimental methodology) is approximately 35 minutes.

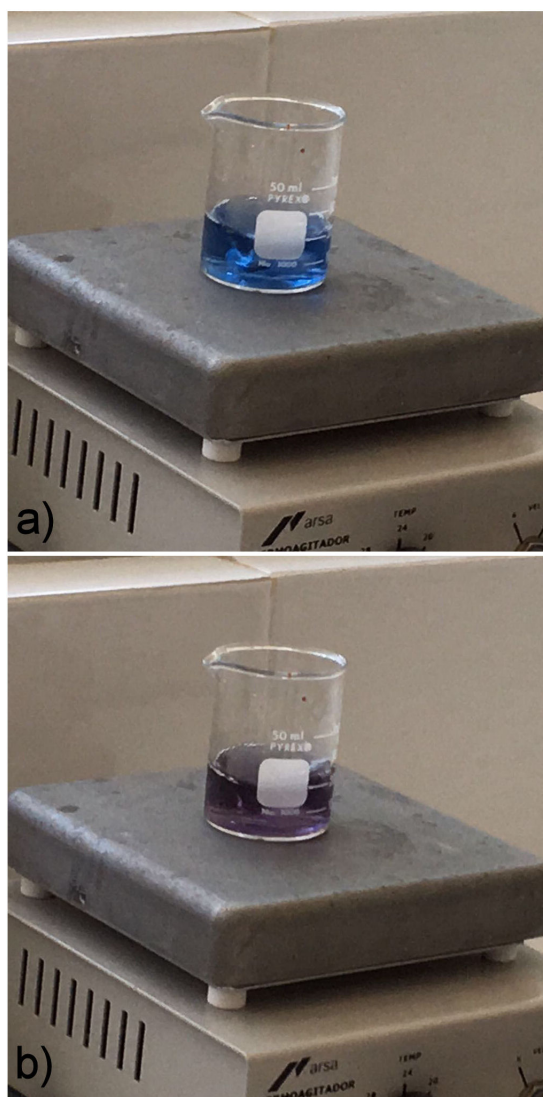


FIGURE 2. Temporary chemical oscillation of the BZ reaction. The color change is caused by changes in the oxidation state of the ferroin indicator. The oscillations of the chemical reaction have a duration of 35 min.

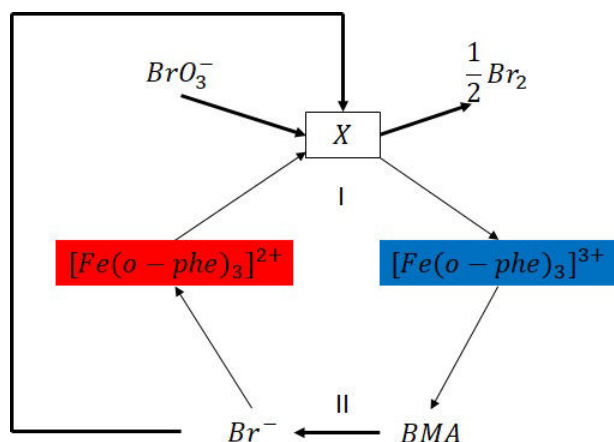


FIGURE 3. The general feedback mechanism of the BZ reaction. Modified from [55].

Essentially, the BZ reaction mechanism consists of two stages, the first one consists in the oxidation of the ferroin indicator by the bromate anion (obtained from the potassium bromate precursor), which gives the solution the blue color. On the other hand, the second stage consists of the reduction of the ferroin indicator in the presence of malonic acid, observing a red coloration in the solution. During the progress of the reaction, the bromate anion allows the production of  $\text{HBrO}_2$ , which facilitates the oxidation process of the indicator. On the other hand, organic compounds derived from bromine (BMA) are formed, which favor the production of bromide ions ( $\text{Br}^-$ ) and reduce the ferroin indicator; however, bromide ions act as strong inhibitors of the feedback mechanism. An outline of the general feedback mechanism can be seen in the Fig. 3 [55].

This process corresponds to a state of self-organization of the system, which results in the emergence of collective properties (oscillations) [48]. The formation of dissipative structures corresponds in the same way to a state of self-organization of the system or self-organized criticality. In this state, the system by itself tends to self-organize without the need for an external disturbance (see Fig. 3) [8,13,25]. The processes of self-organization are present in a great variety of biological systems. The oscillations of concentrations of chemical species are observed in processes such as the hormonal regulation of the thyroid [5], the insulin-leptin axis [36], which is essential for the blood glucose regulation [20], hormone regulation in the menstrual cycle in mammals [49], etc. Disturbances in such oscillatory physiological processes lead to the emergence of pathologies [35]. On the other hand, dissipative structures (spatiotemporal patterns) appear in biological phenomena, such as the formation of patterns in the skin of mammals and fish [30], formation of bacterial colonies [6], crop growth [54] etc.

The numerical solution of the Eqs. (18)-(19) reproduces the oscillatory behavior of the BZ reaction (see Fig. 4a). In Fig. (4b), it is clear that these oscillations emerge due to the existence of a limit cycle in the phase space of variables [16]. In the limit cycle orbits or system solutions of Eqs. (18)-(19)

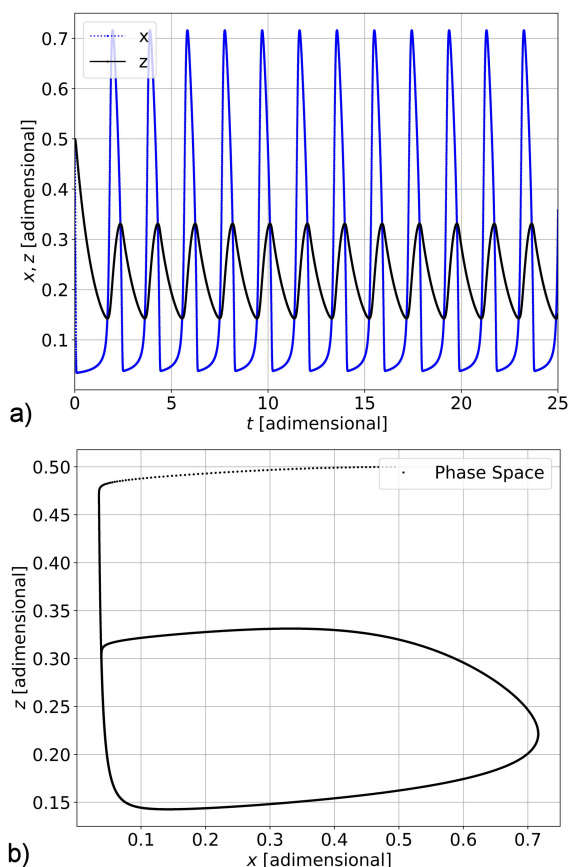


FIGURE 4. Graphs obtained from the numerical solution of the Eqs. (18)-(19). a) Oscillations of the variables  $x$   $y$   $z$  due to the change in the oxidation state of the ferroin indicator. b) Phase space of the variables  $x$  and  $z$ , the presence of a limit cycle is observed [48].

revolve around a fixed point, equilibrium point, or steady-state. The Eqs. (18)-(19) only qualitatively explain the dynamics of the BZ reaction, that is, they explain only the existence of oscillations. However, it is important to note that the Eqs. (18)-(19) can be modified to explain in more detail the dynamics of the BZ reaction [26,1].

In Figs. (5b)-(5c) appears the numerical solution of the Eqs. (20)-(21). The formation of spatio-temporal patterns which corresponds to what was observed in the experimental reproduction of the BZ reaction (see Fig. 5a). However, it is necessary to mention that Eqs. (20)-(21) only qualitatively explain the spatial-temporal dynamics of the BZ reaction, and the spatio-temporal patterns that emerge from the dynamics of the BZ reaction [51].

During the development of the methodology, the student will be able to construct knowledge systemically and integrally, addressing a real problem and implementing tools of Chemistry, Physics, Biology, Mathematics, and Computing. This methodology will allow students to pose new questions and hypotheses It will give them the possibility to explore and build knowledge in a creative way. Besides, the teacher could propose new questions to motivate the creative learning of

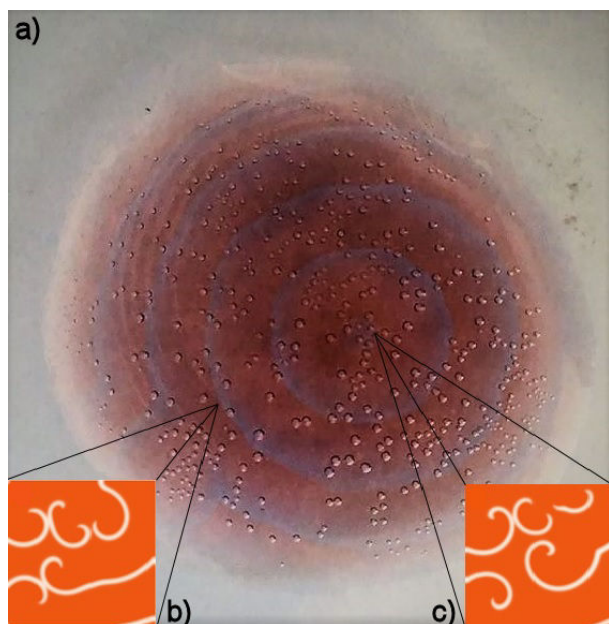


FIGURE 5. a) Formation of chemical waves in the BZ reaction in the absence of agitation. b), c). Numerical solution of the Eqs. (20) - (21). Showing the formation of chemical waves.

the students. Here we propose some topics that may be of interest during the development of the methodology.

- What could happen if the concentration of sulfuric acid in the medium is changed?
- How could the action of pH modify the dynamics of Eqs. (18)-(19)?
- The concentration of sulfuric acid could influence the formation of spatio-temporal patterns?
- If you change the concentration of potassium bromate and potassium bromide, would you modify the frequency of the oscillations?
- What happens if the agitation in the beaker is removed during the chemical reaction?
- Is it possible to observe the formation of chemical waves in 3D during the experimental procedure? If this is possible, what variable has to be modified to observe chemical waves?
- It can be considered that the beaker is a "Batch" type reactor. How could a continuous system (CSTR) be implemented? How would the system of Eqs. (18)-(19)? What parameters would have to be added to the model? How would you modify the dynamics of the model?

$$\frac{dx}{dt} = F(x, z, q, \epsilon, f, flows, volume) \quad (22)$$

$$\frac{dz}{dt} = G(x, z, flows, volume) \quad (23)$$

- The system of Eqs. (18)-(19) arises from a material balance considering the system as a Batch reactor. Is it possible to build an energy balance for the system to study the system temperature ( $T$ )? How would the system of Eqs. (18)-(19)?

$$\frac{dx}{dt} = F(x, z, T, q, \epsilon, f, flows, volume) \quad (24)$$

$$\frac{dz}{dt} = G(x, z, T, flows, volume) \quad (25)$$

$$\frac{dT}{dt} = H(x, z, T, q, \epsilon, f, flows, volume). \quad (26)$$

- How do the dynamics of the Eqs. (18)-(19), if the variables and parameters of the initial conditions model are modified? Modify the Python program of the Euler numeric method.
- How is the dynamic of the Eqs. (20)-(21), if the value of the dimensionless diffusion coefficient is changed? If this parameter is modified, are we still observing spatio-temporal patterns?
- Can the codes built in Python be used to solve numerically other kinetic models?
- The teacher can use the methodology proposed in this paper to propose the theoretical, computational, and experimental study of other oscillating reactions, such as:

- Alternator [37].
- Explodator [31].
- Brusselator [33].
- Berlinator [31].
- Braylator [43].

- Why did Belousov and Zhabotinsky implement the BZ reaction as a strategy to study glycolysis and the Krebs cycle, respectively? What substance in the BZ reaction is used as a chemical species analogous to citric acid?
- Students at more advanced levels can perform the linear stability analysis of eqs. (18) - (21) to study how system dynamics change when one or more parameters of the model are modified (see Fig. 6) [48]. Students will find that the Oregonator model presents a Hopf-Andronov bifurcation [48], and when the Eqs. (18)-(19) are modified, the presence of bistability, hysteresis, and chaos is observed [40,38,52,12,45].
- The teacher can create interactive scripts using the ipywidgets library ([www.ipywidgets.readthedocs.io/en/latest/index.html](http://www.ipywidgets.readthedocs.io/en/latest/index.html)). Below is an example of an interactive script for solving the Eqs. (18)-(19).

- A function that contains the Euler numerical method for the solution of the Eqs. (18)-(19). Once the script is built, it will be saved with the name *bz.py*:



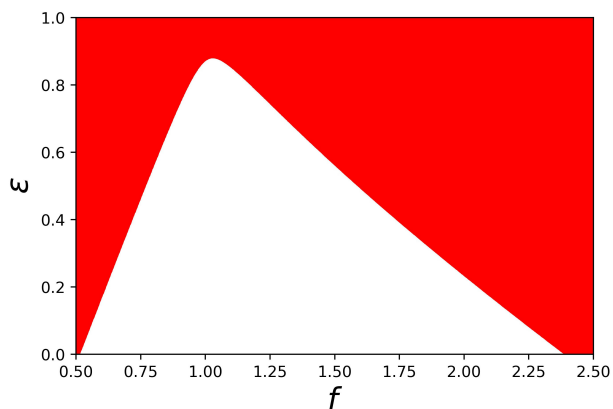


FIGURE 6. Parameter space obtained from the linear stability analysis [48] ( $q = 0.0008$ ). White and red regions show limit cycles and damped oscillations, respectively.

```
In [ ]: #Import modules
import numpy as np
import matplotlib.pyplot as plt
#Function for solve of eqs. (18)-(19)
def solve_bz(f,q,e):
    #Parameters will be find
    #in interactive mode
    f=f
    q=q
    e=e
    #Numerical method parameters
    t0=0.0
    tf=100.0
    dt=0.001
    #Initial condition
    X0=0.5
    Z0=0.5
    #Eqs. (18)-(19)
    def fun1(x,z):
        return (x*(1-x)
        +f*z*((q-x)/(q+x)))/e
    def fun2(x,z):
        return x-z

    #Lists for data
    X=[] #List for x variable
    Z=[] #List for z variable
    T=[] #List for time

    #Assign initial condition
    x=X0
    z=Z0
    #Numerical method
    for t in np.arange(t0,tf,dt):
        t=t+dt
        #Euler rule for x
        x=fun1(x,z)*dt+x
        #Euler rule for z
        z=fun2(x,z)*dt+z
```

```
#list for x values
X.append(x)
#list for z values
Z.append(z)
#list for time values
T.append(t)
```

```
#Plot construction
plt.figure()
plt.plot(T,X,label='x')
plt.plot(T,Z,label='z')
plt.xlabel('t')
plt.ylabel('x,z')
plt.legend(loc='best')
plt.show()
plt.figure()
plt.plot(X,Z,label='PS')
plt.xlabel('x')
plt.ylabel('z')
plt.legend(loc='best')
plt.show()
return [T,X,Z]
#The function returns
#x, z and t values
```

- Later, a script is created that has the instructions of the interactive mode, which must be saved in the same folder as the *bz.py* script:

```
In [ ]: #Import modules
%matplotlib inline
from ipywidgets import
interactive
#Interactive mode module
from bz import solve_bz
#Calling the function above
int=interactive(solve_bz,
f=(0,5.0),q=(0.015,1.0),
e=(0.03,1.0))
int
```

Figures (7)-(8) shows the numerical solution of the Eqs. (18)-(19) for different values of the parameters of the model using the interactive mode. In interactive mode, students can easily modify parameter values and observe the change in system dynamics. The teacher can use the previous script to study the dynamics of other kinetic models [37,31,33,43].

- The proposed methodology can be used to explain to students the relationship that exists between different areas of knowledge. Students must understand that each of the different areas of science are interrelated.

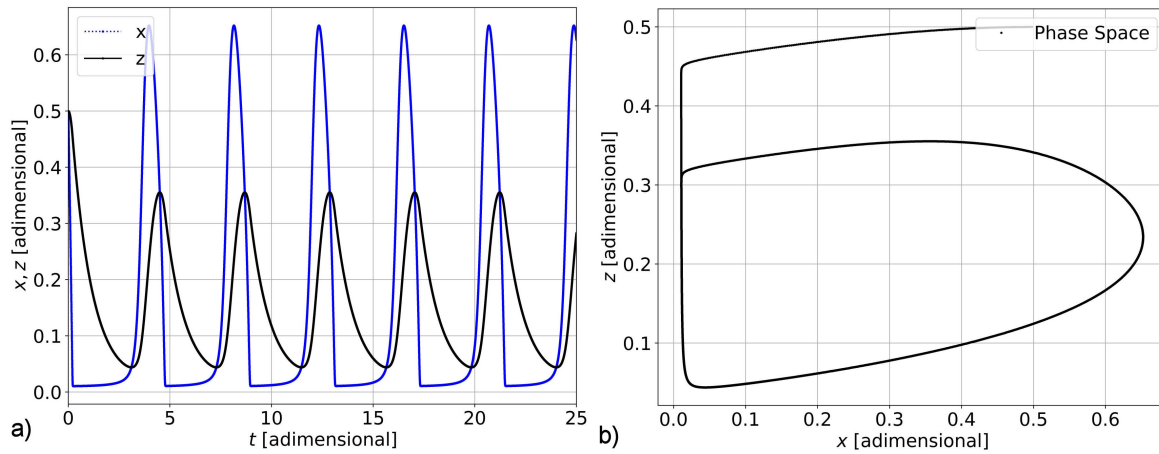


FIGURE 7. Numerical solution of the eqs. (18) - (19) with  $f = 1.0$ ,  $q = 0.015$  and  $\epsilon = 0.11$ . a) Periodic oscillations of the variables  $x$  and  $z$ . b) Phase space, showing a limit cycle [48].

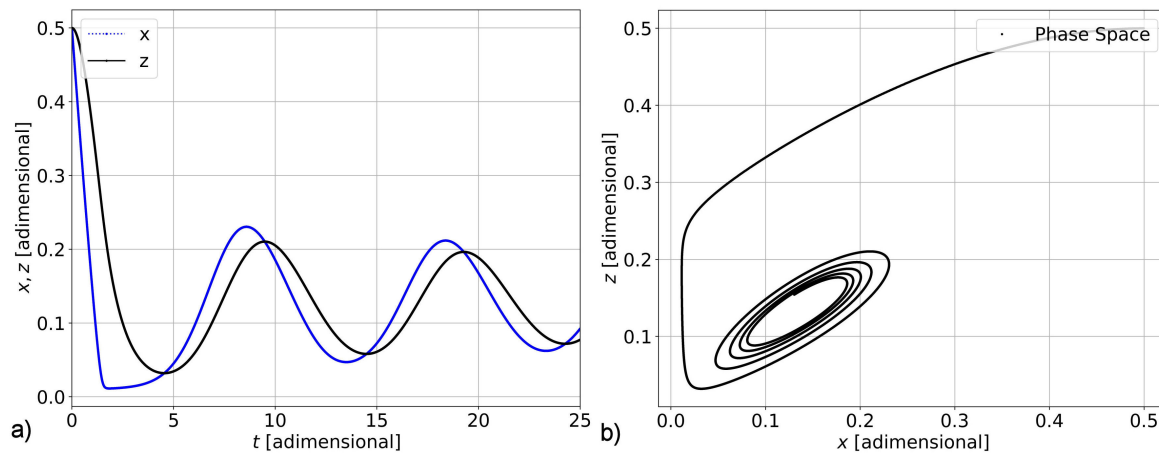


FIGURE 8. Numerical solution of the Eqs. (18)-(19) with  $f = 1.0$ ,  $q = 0.015$  and  $\epsilon = 0.61$ . a) Damped oscillations of the variables  $x$  and  $z$ . b) Phase space. The dynamics of the system changes as a result of the fixed point [48].

## 4. Conclusion

The BZ reaction is one of the ideal prototypes for the application of STEM studies because it allows the implementation and combination of different areas of science (Biology, Chemistry, Physics, Mathematics, and Computing). During the development of the methodology, students will systematically build knowledge understand that the different areas of science are interrelated and that solving or proposing solutions to a real problem requires an interdisciplinary approach. It is of vital importance that the teaching of science allows students to explore and learn actively, eliminating the traditional forms of teaching, in which students only acquire knowledge passively.

## Appendix

### A. Diffusion terms and numerical expressions of them

These systems can be constructed from a generalized conservation law in which, if a differential volume  $V$  surrounded by

a closed surface  $S$  is filled with a substance whose concentration or density is  $x$ , then the rate of change of all substance in  $V$  will be given by a net flux into or from the volume  $V$  across the surface  $S$  and by possible sources or sinks due to reactions or another physical, chemical or biological processes into the volume  $V$ . In this way

$$\frac{dX}{dt} = \frac{d}{dt} \int_V x dv = - \oint_S \vec{J} \cdot d\vec{s} + \int_V f(x, \dots) dv. \quad (\text{A.1})$$

In last expression,  $f(x, \dots)$  represents sources, sinks, reactions (as in this case), dead or born, etc. in the system.

On the other hand, inert matter generally satisfies the empirical Fick's law  $\vec{J}(x) = -D\nabla x$ , where  $D$  is the diffusion coefficient [39]. So that replacing  $\vec{J}(x)$  and applying the divergence theorem in Eq. (A.1):

$$\int_V \frac{dx}{dt} dv = \int_V D\nabla^2 x dv + \int_V f(x, \dots) dv, \quad (\text{A.2})$$

which is valid for any arbitrary volume  $V$ , so that, finally

$$\frac{dx}{dt} = D\nabla^2 x + f(x, \dots), \quad (\text{A.3})$$

is the Reaction-Diffusion Equation, and the function  $f$ , in this case, depends on  $x$ ,  $z$ , and some set of parameters such as reaction velocities or reaction constants.

A numerical expression is necessary for the Laplacian operator  $\nabla^2$ , and it can be obtained from Taylor's series of  $u(x, y)$  around  $x_0$  with small  $h$  as

$$u(x_0 + h, y) = u(x_0, y) + h \frac{\partial u}{\partial x} \Big|_{x_0} + \frac{h^2}{2!} \frac{\partial^2 u}{\partial x^2} \Big|_{x_0} + \dots \quad (\text{A.4})$$

and

$$u(x_0 - h, y) = u(x_0, y) - h \frac{\partial u}{\partial x} \Big|_{x_0} + \frac{h^2}{2!} \frac{\partial^2 u}{\partial x^2} \Big|_{x_0} - \dots \quad (\text{A.5})$$

The sum of Eqs. (A.4) and (A.5) gives

$$u(x_0 + h, y) + u(x_0 - h, y) = 2u(x_0, y) + h^2 \frac{\partial^2 u}{\partial x^2} \Big|_{x_0} + O(h^4), \quad (\text{A.6})$$

which, dividing by  $h^2$  gives an expression for the second partial derivative of  $u(x, y)$  at  $x_0$ , for any  $y$ :

$$\frac{\partial^2 u}{\partial x^2} \Big|_{x_0} = \frac{u(x_0+h) + u(x_0-h) - 2u(x_0)}{h^2} + O(h^2), \quad (\text{A.7})$$

so, if we represent  $u$  using a mesh such that  $u_{ij}$  represents  $u(x, y)$  in a surface element of size  $h^2$ , then the discrete version of the second derivative will be

$$\frac{\partial^2 u_{ij}}{\partial x^2} = \frac{u_{i,j+1} + u_{i,j-1} - 2u_{ij}}{h^2}, \quad (\text{A.8})$$

with an error of  $O(h^2)$  order, and the Laplacian operator is

$$\nabla^2 u_{ij} = \frac{u_{i,j+1} + u_{i,j-1} + u_{i+1,j} + u_{i-1,j} - 4u_{ij}}{h^2}. \quad (\text{A.9})$$

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