Mechanics — *Influence of diffusion on the stability of a full Brusselator model*, by
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Abstract. — The classic Brusselator model consists of four reactions involving six components A,
B, D, E, X, Y. In a typical run, the final products D and E are removed instantly, while, the concentrations of the reactants A and B are kept constant. Then, the classic Brusselator model consisting of
two equations for the intermediate X and Y is obtained. When the component B is not considered
constant, it is added to the mixture and the so-called full Brusselator model is considered. In this
paper, the full Brusselator model is studied. In particular, the boundedness of solutions and the effect
of diffusion on the linear stability is analyzed. Moreover, sufficient conditions ensuring that the
unique steady state, unstable (stable) in the ODEs system, becomes stable (unstable) in presence of
diffusion, are performed and a first nonlinear stability result is obtained.

Key words: Reaction-diffusion systems, Brusselator model, stability, Turing instability

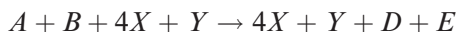Mathematics Subject Classification: 35K57, 35B35, 35B36, 35B40, 35B45

1. Introduction

It is well known that reaction and diffusion of chemical or biochemical species
can produce a variety of spatial patterns. This class of reaction diffusion systems
includes some significant pattern formation equations arising from the modeling
of kinetics of chemical or biochemical reactions and from the biological pattern
formation theory. In this group, the Brusselator model is typically important and
serves as mathematical model in physical chemistry and in biology. Nonlinear
reaction-diffusion equations and systems play an important role in the modeling
and study of many phenomena ([15]–[17] and references therein). Historically, the
Brussels school led by the renowned physical chemist and Nobel Prize laureate
(1977), Ilya Prigogine, made remarkable contributions in the research of complexity of cubic auto-catalytic reactions. The mathematical model signifying their
seminal work was named as the Brusselator (the name was coined by Tyson),
which is originally a system of two ordinary differential equations [7]. The classic
Brusselator model is a famous model of chemical reactions with oscillations and
a theoretical model for a type of auto-catalytic reaction [8]. In particular, the
Brusselator model consists of four reactions involving six-components A, B, D,
E, X, Y where the chemical reactions follow the scheme

$$(1) \qquad \begin{aligned} A &\to X, \\ B + X &\to Y + D, \end{aligned}$$

$$2X + Y \to 3X,$$
$$X \to E.$$
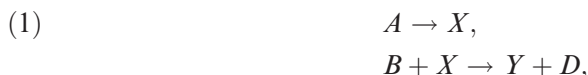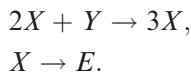
Adding these reactions one obtains

$$A + B + 4X + Y \to 4X + Y + D + E$$

and hence $A + B \to D + E$ then, X and Y are catalysis (in particular, $(1)_3$ shows that X is auto-catalytic and provides the nonlinearity). There are several known examples of auto-catalysis which can be modeled by the Brusselator equations, such as ferrocyanide-iodate-sulphite reaction, chlorite-iodite-malonic acid reaction, arsenite-iodate reaction, some enzyme catalytic reactions and fungal mycelia growth [21]–[23], [27]. In a typical run, the final products D and E are removed instantly since they do not affect the reaction kinetics, while, the reactant concentrations are kept in excess and, if A and B are held constant during the reaction process, all the concentrations are fixed quantities. In this case it is coming to a system of two equations for intermediates X and Y, and hence the well-known binary Brusselator model is obtained. This is when it is realistic to assume all the reactant concentrations to be constant [5, 29]. When the component B is not considered constant and it is added to the mixture with a constant rate α, the so-called full Brusselator model is considered [28]. The behavior of the full model differs substantially from that of the simplified model but in literature we have not seen many advancing results [20, 24, 28]. In 1993 two consecutive papers [25, 26], discovered a variety of interesting self-replicating pattern formation associated with cubic-autocatalytic reaction-diffusion systems, respectively by an experimental approach and a numerical simulation approach. Since then numerous studies by mathematical and computational analysis have shown that the cubic-autocatalytic reaction-diffusion systems such as Brusselator equations and Gray–Scott equations [18]–[19] exhibit rich spatial patterns (for instance Turing patterns) and complex bifurcations as well as interesting dynamics. For this reason, the Brusselator model has been widely studied and many properties of it had been researched by many people via different methods (see for instance [9]–[14] and reference therein). To make theory more realistic, for Brusselator equations and other cubic-autocatalytic equations, extended systems [2]–[4], [6] (just to give an idea, six coupled components with partial reversibility, forced systems) have been introduced, and dynamics more challenging and cumbersome have been shown. In the present paper, we consider the full Brusselator model, introduced in [28], aimed to investigate for the effect of diffusion on the stability of the (unique) constant steady state. The plan of the paper is as follows. Section 2 is devoted to the introduction of the mathematical model. The boundedness of solutions is proved in Section 3 while the existence of meaningful equilibria is analyzed in Section 4. Linear stability analysis is performed in Section 5 where, in particular, both the stabilizing or destabilizing effect of diffusion have been highlighted. Nonlinear stability analysis is investigated in Section 6. The paper ends with Section 7 in which the model is analyzed under Robin boundary condi-

tions and the stability of the meaningful equilibrium is investigated via numerical simulations.

2. Preliminaries

This paper deals with the full Brusselator reaction-diffusion model governing the evolution of X, Y, and B in (1) under the hypotheses of unit reaction rates, A kept in excess ($A = 1$) and B added to the mixture with a constant rate $\alpha > 0$ [28]. Denoting by X_i, ($i =, 1, 2, 3$), the concentrations of X, Y, B, respectively, the model is given by

$$(2) \quad \begin{cases} X_{1,t} = 1 + X_1^2 X_2 - X_1 X_3 - X_1 + \gamma_1 \Delta X_1, \\ X_{2,t} = X_1 X_3 - X_1^2 X_2 + \gamma_2 \Delta X_2, \\ X_{3,t} = -X_1 X_3 + \alpha + \gamma_3 \Delta X_3, \end{cases}$$

where $\gamma_i = \text{const.} > 0$ ($i = 1, 2, 3$) denotes the diffusion coefficients of X_i and $X_{i,t}$, ($i = 1, 2, 3$), denotes the partial time derivative of X_i. As concerns model (2) it should be remarked that, from a mathematical point of view, it appears that for $X_3 = \text{const.}$, (2) does not reduce to the classic binary Brusselator model ([17], [19]). This is because the chemical reaction with X_3 not kept in excess (i.e. X_3 not constant) leads to a model involving the kinetics of X_3 which is different from the binary Brusselator model. Denoting by D the bounded, connected, open subset of R^3 in which chemical reaction occurs, we assume that D has a Lipschitz boundary ∂D and $X_i : (\mathbf{x}, t) \in D \times [0, \infty] \to X_i(\mathbf{x}, t) \in \mathbb{R}^+$, $X_i \in W^{1,2}(D)$, ($i = 1, 2, 3$). To (2) we append the following smooth positive initial data

$$(3) \quad X_i(\mathbf{x}, 0) = X_i^0(\mathbf{x}), \quad \text{in } D, \quad (i = 1, 2, 3)$$

with $X_i^0 \in C(\overline{D})$ and the Robin boundary conditions

$$(4) \quad \beta_i X_i + (1 - \beta_i)\nabla X_i \cdot \mathbf{n} = \beta_i \overline{X}_i, \quad \text{on } \partial D \times \mathbb{R}^+,$$

being $\mathbf{n}$ the outward unit normal to ∂D, $\beta_i \in (0, 1)$, ($i = 1, 2, 3$) and $\overline{X}_i = \text{const.} > 0$ assigned ($i = 1, 2, 3$). Boundary conditions (4) are the more general ones that can be added to (2). However, in view of the chemistry of the problem under consideration, since X_i ($i = 1, 2$) are catalytic in reaction (1) while X_3 is consuming, it appears more appropriate to assume that: 1) there is no-flux at boundary for X_1 and X_2; 2) X_3 is introduced into the chemical reaction from the outside at a constant rate. This leads to assume in (4) $\beta_i = 0$ ($i = 1, 2$), $\beta_3 = \beta \in (0, 1)$ and hence to consider the following boundary conditions:

$$(5) \quad \begin{cases} \nabla X_i \cdot \mathbf{n} = 0, \quad \text{on } \partial D \times \mathbb{R}^+, \quad (i = 1, 2), \\ \beta X_3 + (1 - \beta)\nabla X_3 \cdot \mathbf{n} = \beta \overline{X}_3, \quad \text{on } \partial D \times \mathbb{R}^+. \end{cases}$$

Due to the relevance in chemical applications, in Sections 3–6 we will perform the dynamics of (2), (3), (5) and – for the sake of completeness – we will analyze the dynamics of (2)–(4) in Section 7, via numerical simulations.

3. BOUNDEDNESS OF SOLUTIONS

In the sequel we will denote by: $\|\cdot\|$, $\|\cdot\|_\infty$, $\|\cdot\|_{\partial D}$ the $L^2(D)$, $L^\infty(D)$ and $L^2(\partial D)$ norm, respectively; $\langle\cdot,\cdot\rangle$ the scalar product in $L^2(D)$; $|D|$ the (finite) measure of D. The following theorem – given by a direct consequence of Theorem 1 of [1] – provides the $L^\infty(D)$-norm estimates for X_i ($i=1,2,3$).

THEOREM 1. *Let (X_1, X_2, X_3) be positive solution of (2)–(5). Then there exist positive constants $C_\infty^{(j)}$ ($j=1,2,3$), depending on the initial data, such that*

(6)
$$\|X_1\|_\infty \le C_\infty^{(1)}, \quad \|X_2\|_\infty \le C_\infty^{(2)}, \quad \|X_3\|_\infty \le C_\infty^{(3)}.$$

PROOF. By virtue of (2), (3), (5), let us consider the following initial-boundary value problem

(7)
$$\begin{cases} X_{3,t} - \gamma_3 \Delta X_3 = -X_1 X_3 + \alpha, & D \times \mathbb{R}^+, \\ \beta X_3 + (1-\beta)\nabla X_3 \cdot \mathbf{n} = \beta \bar{X}_3, & \partial D \times \mathbb{R}^+, \\ X_3(\mathbf{x}, 0) = X_3^0(\mathbf{x}), & D. \end{cases}$$

Since

(8)
$$-X_1 X_3 + \alpha < \frac{X_3^2}{2} + \alpha,$$

in view of Theorem 1 of [1], choosing $p_0 = 2$, one obtains that, denoting by $\tau(X_3^0)$ the maximal existence time of the solution X_3 of (7), since – from the continuous dependence on the initial data – there exists a positive constant $C_3(X_3^0)$ such that

(9)
$$\|X_3(\cdot, t)\| \le C_3(X_3^0), \quad \forall t \in (0, \tau(X_3^0)),$$

the solution X_3 exists for all time and there exists a positive constant C_∞ such that

(10)
$$\|X_3(\cdot, t)\|_\infty \le C_\infty^{(3)}(X_3^0), \quad \forall t > 0.$$

Now let us multiply equation $(2)_2$ by X_2, then on applying Young inequality, one obtains:

(11)
$$\frac{\partial X_2^2}{\partial t} \le -X_1^2 X_2^2 + X_3^2 + \gamma_2 \Delta(X_2^2)$$

and hence X_2^2 is a sub-solution of the following initial-boundary value problem:

(12)
$$\begin{cases} Y_{2,t} - \gamma_2 \Delta Y_2 = X_3^2, & D \times \mathbb{R}^+, \\ \nabla Y_2 \cdot \mathbf{n} = 0, & \partial D \times \mathbb{R}^+, \\ Y_2(\mathbf{x}, 0) = Y_2^{(0)}(\mathbf{x}) = \max_{\bar{D}}(X_2^0(\mathbf{x}))^2, & D. \end{cases}$$

Since

(13) $$X_3^2 < (C_\infty^{(3)})^2 + c_1 Y_2^2, \quad c_1 = \text{const.} > 0, \quad \text{a.e. in } D$$

in view of Theorem 1 of [1], choosing $p_0 = 2$, one obtains that, denoting by $\tau_1(Y_2^0)$ the maximal existence time of the solution Y_2 of (12), since – from the continuous dependence on the initial data – there exists a positive constant $C_2(Y_2^0)$ such that

(14) $$\|Y_2(\cdot, t)\| \leq C_2(Y_2^0), \quad \forall t \in (0, \tau_1(Y_2^0)),$$

the solution Y_2 exists for all time and there exists a positive constant $\tilde{C}_\infty^{(2)}$ such that

(15) $$\|Y_2(\cdot, t)\|_\infty \leq \tilde{C}_\infty^{(2)}, \quad \forall t > 0.$$

Hence, since X_2^2 is a sub-solution of (12), one obtains:

(16) $$\|X_2^2(\cdot, t)\|_\infty \leq \|Y_2(\cdot, t)\|_\infty \leq \tilde{C}_\infty^{(2)}, \quad \forall t > 0.$$

From (16), then $(6)_2$ is immediately obtained.

Finally let us consider the following initial-boundary value problem

(17) $$\begin{cases} X_{1,t} - \gamma_1 \Delta X_1 = 1 + X_1^2 X_2 - X_1 X_3 - X_1, & D \times \mathbb{R}^+, \\ \nabla X_1 \cdot \mathbf{n} = 0, & \partial D \times \mathbb{R}^+, \\ X_1(\mathbf{x}, 0) = X_1^0(\mathbf{x}), & D. \end{cases}$$

Since

(18) $$|1 + X_1^2 X_2 - X_1 X_3 - X_1| \leq \left(C_\infty^{(2)} + \frac{C_\infty^{(3)} + 1}{2}\right) X_1^2 + \left(1 + \frac{C_\infty^{(3)} + 1}{2}\right)$$

in view of Theorem 1 of [1], choosing $p_0 = 2$, one obtains that, denoting by $\tau_1(X_1^0)$ the maximal existence time of the solution X_1 of (17), since – from the continuous dependence on the initial data – there exists a positive constant $C_1(X_1^0)$ such that

(19) $$\|X_1(\cdot, t)\| \leq C_1(X_1^0), \quad \forall t \in (0, \tau_1(X_1^0)),$$

the solution X_1 exists for all time and there exists a positive constant $C_\infty^{(1)}$ such that

(20) $$\|X_1(\cdot, t)\|_\infty \leq C_\infty^{(1)}, \quad \forall t > 0.$$

REMARK 1. We remark that, in view of (6), there exist positive constants M_1, M_2, M_3 such that

(21) $$\|X_1\|^2 \leq M_1, \quad \|X_2\|^2 \leq M_2, \quad \|X_3\|^2 \leq M_3.$$

4. CONSTANT EQUILIBRIA AND PRELIMINARIES TO STABILITY

The unique non negative constant solution $\bar{E}(\bar{X}_1, \bar{X}_2, \bar{X}_3)$ of (2), (5) (constant steady state) is given by $\bar{E} = (1, \alpha, \alpha)$. Setting $\{u = X_1 - 1,\ v = X_2 - \alpha,\ w = X_3 - \alpha\}$, the system governing the evolution of the perturbation fields is

$$(22) \qquad \begin{cases} u_t = -(1 - \alpha)u + v - w + \gamma_1 \Delta u + F_1(u, v, w), \\ v_t = -\alpha u - v + w + \gamma_2 \Delta v + F_2(u, v, w), \\ w_t = -\alpha u - w + \gamma_3 \Delta w + F_3(u, v, w), \end{cases}$$

with $F_i(u, v, w)$ non-linear terms given by:

$$(23) \qquad F_1 = \alpha u^2 + u^2 v + 2uv - uw, \quad F_2 = -F_1, \quad F_3 = -uw.$$

To (22) we associate the boundary conditions

$$(24) \quad \nabla u \cdot \mathbf{n} = 0, \quad \nabla v \cdot \mathbf{n} = 0, \quad \beta w + (1 - \beta)\nabla w \cdot \mathbf{n} = 0, \quad \text{on } \partial D \times \mathbb{R}^+,$$

with $\beta \in (0, 1)$.

We denote by [17]:

- $H^1(D, \beta)$ the functional space such that

$$\Phi \in H^1(D, \beta) \Rightarrow \{\Phi^2 + (\nabla \Phi)^2 \in L^1(D), \beta \Phi + (1 - \beta)\nabla \Phi \cdot \mathbf{n} = 0, \text{ on } \partial D\};$$

- $\bar{\mu} = \bar{\mu}(D)$ the lowest eigenvalue of the spectral problem

$$(25) \qquad \begin{cases} \Delta \Phi + \mu \Phi = 0 & \text{in } D, \\ \beta \Phi + (1 - \beta)\nabla \Phi \cdot \mathbf{n} = 0 & \text{on } \partial D \end{cases}$$

  with $\Phi \in H^1(D, \beta)$;
- $\{\Phi_n\}_{n \in \mathbb{N}}$ an orthogonal complete sequence of eigenfunctions of (25) with eigenvalues $\{\mu_n\}_{n \in \mathbb{N}}$ such that [31]:

$$(26) \qquad 0 < \bar{\mu} = \mu_1 < \mu_2 \leq \cdots \leq \mu_n \leq \cdots$$

As it is well known, $\forall \Phi \in H^1(D, \beta)$ the following inequality holds [17]:

$$(27) \qquad \|\nabla \Phi\|^2 + \frac{\beta}{1 - \beta}\|\Phi\|_{\partial D}^2 \geq \bar{\mu}\|\Phi\|^2.$$

For $\beta = 0$ one obtains

$$H^1(D, 0) = \{\Phi^2 + (\nabla \Phi)^2 \in L^1(D), \nabla \Phi \cdot \mathbf{n} = 0, \text{ on } \partial D\}$$

and, in this case, on denoting by $\{\Phi_n\}_{n \in \mathbb{N}}$ an orthogonal complete sequence of eigenfunctions of the spectral problem:

$$(28) \qquad \begin{cases} \Delta\Phi + \sigma\Phi = 0 & \text{in } D, \\ \nabla\Phi \cdot \mathbf{n} = 0 & \text{on } \partial D, \end{cases}$$

the eigenvalues $\{\sigma_n\}_{n \in \mathbb{N}}$ are such that

$$(29) \qquad 0 = \sigma_1 < \sigma_2 \le \sigma_3 \le \cdots \le \sigma_n \le \cdots$$

Denoting by $\mathscr{J}$ the Jacobian matrix associated to (22), for each $i = 1, 2, 3, \ldots, \lambda$ is an eigenvalue of $\mathscr{J}$ if and only if λ is an eigenvalue of the matrix

$$(30) \qquad \tilde{\mathscr{J}}_i = \begin{pmatrix} \alpha - 1 - \sigma_i\gamma_1 & 1 & -1 \\ -\alpha & -1 - \sigma_i\gamma_2 & 1 \\ -\alpha & 0 & -1 - \mu_i\gamma_3 \end{pmatrix}.$$

The characteristic equation of $\tilde{\mathscr{J}}_i$ is

$$(31) \qquad \lambda_i^3 - I_{1i}\lambda_i^2 + I_{2i}\lambda_i - I_{3i} = 0,$$

where I_{ji}, $(j = 1, 2, 3)$, are the principal $\tilde{\mathscr{J}}_i$-invariants given by

$$(32) \qquad \begin{cases} I_{1i} = I_1^0 - (\gamma_1 + \gamma_2)\sigma_i - \gamma_3\mu_i, \\ I_{2i} = I_2^0 + \gamma_1\gamma_2\sigma_i^2 + \gamma_3(\gamma_1 + \gamma_2)\sigma_i\mu_i + [2(\gamma_1 + \gamma_2) - \alpha\gamma_2]\sigma_i + (2 - \alpha)\gamma_3\mu_i, \\ I_{3i} = I_3^0 - \gamma_1\gamma_2\gamma_3\sigma_i^2\mu_i - \gamma_1\gamma_2\sigma_i^2 + \gamma_3[\alpha\gamma_2 - (\gamma_1 + \gamma_2)]\sigma_i\mu_i \\ \qquad + [2\alpha\gamma_2 - (\gamma_1 + \gamma_2)]\sigma_i - \gamma_3\mu_i, \end{cases}$$

with I_j^0, $(j = 1, 2, 3)$, being the principal invariants of the linear operator in the absence of diffusion, i.e.

$$(33) \qquad I_1^0 = \alpha - 3, \quad I_2^0 = 3 - 2\alpha, \quad I_3^0 = -1.$$

The necessary and sufficient conditions guaranteeing that all the roots of (31) have negative real part and hence that $\bar{E}$ is linearly stable are the Routh–Hurwitz conditions [30]:

$$(34) \qquad I_{1i} < 0, \quad I_{3i} < 0, \quad I_{1i}I_{2i} - I_{3i} < 0, \quad \forall i \in \mathbb{N}$$

being

$$(35) \quad I_{1i}I_{2i} - I_{3i} = -\gamma_1\gamma_2(\gamma_1 + \gamma_2)\sigma_i^3 - \gamma_3(\gamma_1 + \gamma_2)^2\sigma_i^2\mu_i +$$
$$- \gamma_3^2(\gamma_1 + \gamma_2)\sigma_i\mu_i^2 - [2\gamma_1^2 + (2 - \alpha)\gamma_2^2 + 2(3 - \alpha)\gamma_1\gamma_2]\sigma_i^2 +$$
$$- 2\gamma_3(\gamma_1 + \gamma_2)(3 - \alpha)\sigma_i\mu_i - [\gamma_2(\alpha^2 - 5\alpha + 8) + 4\gamma_1(2 - \alpha)]\sigma_i$$
$$+ (\alpha - 2)\gamma_3^2\mu_i^2 - (\alpha^2 - 7\alpha + 8)\gamma_3\mu_i + I_1^0 I_2^0 - I_3^0.$$

Let us underline that conditions (34) imply necessarily that

$$
(36) \qquad\qquad l_{2i} > 0, \quad \forall i \in I\!N.
$$

Vice-versa if there exists at least one $\bar{i} \in \{1, 2, \ldots\}$ such that at least one of (34) or (36) is not verified, then instability of $\bar{E}$ occurs.

5. Effect of diffusion on linear stability

In this Section we perform the linear stability analysis of the null solution of (22)–(24). Furthermore, we investigate for the stabilizing/destabilizing effect of diffusion comparing the linear stability results to those ones obtained in the absence of diffusion. In particular, we will prove sufficient conditions guaranteeing the stabilizing effect of diffusion and sufficient conditions guaranteeing that Turing instability (i.e. diffusion driven instability) occurs. The following theorems hold true.

THEOREM 2. *In the absence of diffusion, the equilibrium $\bar{E}$ is linearly stable if and only if*

$$
(37) \qquad\qquad \alpha < \frac{9 - \sqrt{17}}{4}.
$$

PROOF. The proof follows by remarking that (37) is necessary and sufficient to guarantee that $\{l_1^0 < 0, l_3^0 < 0, l_1^0 l_2^0 - l_3^0 < 0\}$.

REMARK 2. We remark that – in the absence of diffusion – when

$$
(38) \qquad\qquad \alpha = \frac{9 - \sqrt{17}}{4},
$$

instability of $\bar{E}$ can occur only via an oscillatory state. In fact (38) implies that the characteristic equation

$$
(39) \qquad\qquad \lambda^3 - l_1^0 \lambda^2 + l_2^0 \lambda - l_3^0 = 0,
$$

admits a real negative root and the pure imaginary roots $\lambda = \pm i\omega$ with

$$
(40) \qquad\qquad \omega^2 = \frac{l_3^0}{l_1^0} = l_2^0 \in \mathbb{R}\backslash\{0\}.
$$

THEOREM 3. *A sufficient condition guaranteeing the instability of $\bar{E}$ is*

$$
(41) \qquad\qquad \alpha \geq 2.
$$

PROOF. In view of $(32)_2$, it follows that (41) implies $I_{21} < 0$, i.e. (36) is not verified for $i = 1$ and hence instability of $\bar{E}$ occurs.

In view of theorem 3, the linear stability analysis of $\bar{E}$ (i.e. in the presence of diffusion), can be reduced to analyze the case $\alpha < 2$.

THEOREM 4. *If either*

$$(42) \qquad \alpha < \min\left\{\frac{\gamma_1 + \gamma_2}{2\gamma_2}, \frac{9 - \sqrt{17}}{4}\right\},$$

or

$$(43) \qquad \begin{cases} \dfrac{9 - \sqrt{17}}{4} < \alpha < \min\left\{\dfrac{\gamma_1 + \gamma_2}{2\gamma_2}, 2\right\}, \quad \dfrac{\gamma_2}{\gamma_1} < \dfrac{2}{7 - \sqrt{17}} \\[2mm] \mu_1 \gamma_3 > \dfrac{-\alpha^2 + 7\alpha - 8 + \sqrt{\alpha(\alpha - 1)(\alpha^2 - 5\alpha + 8)}}{2(2 - \alpha)}, \end{cases}$$

then $\bar{E}$ is linearly stable.

PROOF. Both in the case (42) and $(43)_1$–$(43)_2$, since in particular $\alpha < 2$, then on accounting for (32) and (35), by simple calculations one immediately verifies that $(34)_1$ and $(34)_2$ are satisfied. Passing to analyze the validity of $(34)_3$, on accounting for (35), it is certainly ensured by condition (42), while if $(43)_1$–$(43)_2$ hold true, $(34)_3$ is verified if

$$(44) \qquad (\alpha - 2)\gamma_3^2\mu_i^2 - (\alpha^2 - 7\alpha + 8)\gamma_3\mu_i + I_1^0 I_2^0 - I_3^0 < 0, \quad \forall i \in I\!N,$$

i.e.

$$(45) \qquad \gamma_3\mu_i > \frac{-\alpha^2 + 7\alpha - 8 + \sqrt{\alpha(\alpha - 1)(\alpha^2 - 5\alpha + 8)}}{2(2 - \alpha)} \quad \forall i \in I\!N$$

which, by virtue of (26), is guaranteed if $(43)_3$ holds true.

REMARK 3. We remark that:

i) (42) implies (37) and hence implies stability in the absence of diffusion too (Turing instability can not occur);
ii) (43) implies that (37) does not hold, i.e. (43) implies instability in the absence of diffusion and stability in the presence of diffusion (stabilizing effect of diffusion).

Let us investigate for the occurrence of Turing instability. Setting

$$(46) \quad \begin{cases} \bar{\gamma}_2 = \dfrac{\gamma_1\sigma_2 + 1}{2\alpha - 1 - \sigma_2\gamma_1}, \quad \bar{\mu}_2 = \dfrac{-1 - \sigma_2(\gamma_1 + \gamma_2) + 2\sigma_2\alpha\gamma_2 - \sigma_2^2\gamma_1\gamma_2}{1 + \sigma_2(\gamma_1 + \gamma_2) - \sigma_2\alpha\gamma_2 + \sigma_2^2\gamma_1\gamma_2}, \\ \delta = \{2\gamma_1\gamma_2 - \gamma_3[\alpha\gamma_2 - (\gamma_1 + \gamma_2)]\}^2 + 8\gamma_1\gamma_2\gamma_3[2\alpha\gamma_2 - (\gamma_1 + \gamma_2)], \\ \tilde{\gamma}_2 = \dfrac{\gamma_1\sigma_2 + 1}{\alpha - 1 - \sigma_2\gamma_1}, \end{cases}$$

the following theorem holds.

THEOREM 5. *If either*

$$(47) \qquad \frac{1}{2} < \alpha \le 1, \quad \gamma_1\sigma_2 < 2\alpha - 1, \quad \sigma_2\gamma_2 > \bar{\gamma}_2, \quad \gamma_3\mu_2 < \bar{\mu}_2,$$

or

$$(48) \quad 1 < \alpha < \frac{9 - \sqrt{17}}{4}, \quad \gamma_1\sigma_2 < \alpha - 1, \quad \bar{\gamma}_2 < \sigma_2\gamma_2 < \tilde{\gamma}_2, \quad \gamma_3\mu_2 < \bar{\mu}_2,$$

or

$$(49) \qquad 1 < \alpha < \frac{9 - \sqrt{17}}{4}, \quad \gamma_1\sigma_2 < \alpha - 1, \quad \sigma_2\gamma_2 > \tilde{\gamma}_2,$$

or

$$(50) \quad 1 < \alpha < \frac{9 - \sqrt{17}}{4}, \quad \alpha - 1 \le \gamma_1\sigma_2 < 2\alpha - 1, \quad \sigma_2\gamma_2 > \tilde{\gamma}_2, \quad \gamma_3\mu_2 < \bar{\mu}_2,$$

then Turing instability occurs.

PROOF. The proof follows by remarking that each one of conditions (47)–(50) implies that (37) holds but $I_{32} > 0$. Hence (34)$_2$ is not verified for $i = 2$ and there is the so-called *diffusion driven instability* (Turing instability). ∎

REMARK 4. Let us remark that there is a destabilizing effect on the unique steady state in generalizing the classic Brusselator model by incorporating the dynamic of B-component in (1). In fact, the classic Brusselator model governing the evolution of X, Y, in (1) under the hypotheses of unit reaction rates, A and B kept in excess ($A = 1$, $B = b = \text{const.} > 0$) is given by

$$(51) \quad \begin{cases} X_{1,t} = 1 + X_1^2 X_2 - bX_1 - X_1 + \gamma_1\Delta X_1, & \text{in } D \\ X_{2,t} = bX_1 - X_1^2 X_2 + \gamma_2\Delta X_2, & \text{in } D \\ \nabla X_i \cdot \mathbf{n} = 0, & \text{on } \partial D \times \mathbb{R}^+. \end{cases}$$

The unique steady state of (51) is $\tilde{E} = (1, b)$ and the perturbation system is

$$(52) \quad \begin{cases} u_t = (b - 1)u + v + F_1 + \gamma_1\Delta u, \\ v_t = -bu - v - F_1 + \gamma_2\Delta v, \end{cases}$$

being $u = X_1 - 1$, $v = X_2 - b$, $F_1 = u^2(b + v) + 2uv$. The invariants of the linear operator associated to (52) are

(53) $\qquad I_{1i}^{(2)} = b - 2 - \sigma_i(\gamma_1 + \gamma_2), \quad I_{2i}^{(2)} = \gamma_1\gamma_2\sigma_i^2 + [\gamma_1 + \gamma_2(1 - b)]\sigma_i + 1$

with σ_i given by (29). Hence $b < 2$ is necessary for the linear stability since $b \geq 2$ implies that $I_{11}^{(2)} > 0$. Simple calculation shows that, if

(54) $$b < \min\left\{1 + \frac{\gamma_1}{\gamma_2}, 2\right\},$$

then $\tilde{E}$ is linearly stable. Concerning the so-called "full Brusselator model", the reactant B is not considered constant and moreover it is added to the mixture with a constant rate $\alpha(> 0)$. Adopting the ansatz that α plays the role of b in model (2), on comparing (54) to (42), it follows that since $\min\left\{\dfrac{9 - \sqrt{17}}{4}, \dfrac{\gamma_1 + \gamma_2}{2\gamma_2}\right\} \leq \min\left\{2, 1 + \dfrac{\gamma_1}{\gamma_2}\right\}$, it is possible – a priori – to find some values of b guaranteeing stability of $\tilde{E}$ and instability of $\bar{E}$. In fact, if $b = \alpha$ and

(55) $$1 < \alpha < \min\left\{\frac{9 - \sqrt{17}}{4}, 1 + \frac{\gamma_1}{\gamma_2}\right\},$$

holds together with (49) one has that $\tilde{E}$ is stable while $\bar{E}$ is unstable. A possible combination of the parameters verifying these conditions is

(56) $$\begin{cases} 1 < \alpha < \dfrac{9 - \sqrt{17}}{4}, \quad \gamma_1 < \dfrac{\alpha - 1}{\sigma_2}, \\ \gamma_2 > \max\left\{\dfrac{4\gamma_1}{5 - \sqrt{17}}, \dfrac{\gamma_1(\gamma_1\sigma_2 + 1)}{(\alpha - 1)(\alpha - 1 - \sigma_2\gamma_1)}\right\}. \end{cases}$$

Further generalization of system (51) can be obtained incorporating both the kinetics of A and B involved in reaction (1). In this way a PDE system governing the dynamic of A, B, X, Y arises and we expect a deeper destabilizing effect on the unique steady state.

6. Nonlinear stability analysis

In this Section we perform the nonlinear stability analysis of $\bar{E}$ with respect to the energy-norm

(57) $$V(t) = \frac{1}{2}[\alpha\|u\|^2 + \|v\|^2 + \|w\|^2].$$

THEOREM 6. *If $\alpha \in (0, 1/3)$ or if*

(58) $$\alpha \in \left(\frac{1}{3}, 1\right), \quad \bar{\mu}\gamma_3 > \frac{3\alpha - 1}{1 - \alpha}$$

with $\bar{\mu}$ the lowest eigenvalue of (25), $\bar{E}$ is nonlinearly (locally) asymptotically stable with respect to the V-norm.

PROOF. The time derivative of V along the solutions of (22)–(24), by virtue of (27), is given by

$$(59) \qquad \dot{V} = \alpha(\alpha - 1)\|u\|^2 - 2\alpha\langle u, w\rangle + \langle v, w\rangle - \|v\|^2 - \|w\|^2 +$$

$$- \alpha\gamma_1\|\nabla u\|^2 - \gamma_2\|\nabla v\|^2 - \gamma_3\|\nabla w\|^2 - \gamma_3\frac{\beta}{1-\beta}\|w\|_{\partial D}^2 + \Phi,$$

being

$$(60) \qquad\qquad \Phi = \alpha\langle u, F_1\rangle + \langle v, F_2\rangle + \langle w, F_3\rangle$$

with F_i $(i = 1, 2, 3)$ given by (23).

In view of generalized Cauchy inequality, one has

$$(61) \qquad \dot{V}(t) \le \alpha\left(\alpha - 1 + \frac{2\alpha}{\varepsilon_1}\right)\|u\|^2 - \frac{1}{2}\|v\|^2 - \frac{1}{2}[1 + \bar{\mu}\gamma_3 - \varepsilon_1]\|w\|^2 +$$

$$- \alpha\gamma_1\|\nabla u\|^2 - \gamma_2\|\nabla v\|^2 - \gamma_3\|\nabla w\|^2 + \Phi.$$

By applying the Sobolev inequality $\|f\|_4^2 \le k(D)[\|\nabla f\|^2 + \|f\|^2]$ and $(6)_2$, it turns out that

$$(62) \qquad \Phi \le c_1(D)(\|u\| + \|v\| + \|w\|)[\|u\|^2 + \|v\|^2 + \|w\|^2 + \|\nabla u\|^2$$

$$+ \|\nabla v\|^2 + \|\nabla w\|^2],$$

with

$$(63) \qquad\qquad c_1(D) = k(D)\max\{\alpha(2\alpha + C_\infty^{(2)}), 3\alpha, 5/2\}.$$

Setting

$$(64) \qquad\qquad k_1 = 2\left(1 - \alpha - \frac{2\alpha}{\varepsilon_1}\right), \quad k_2 = 1 + \bar{\mu}\gamma_3 - \varepsilon_1,$$

substituting (62) into (61), it turns out that

$$(65) \qquad \dot{V}(t) \le -\frac{\alpha k_1}{2}\|u\|^2 - \frac{\|v\|^2}{2} - \frac{k_2}{2}\|w\|^2 - \min\{\alpha\gamma_1, \gamma_2, \gamma_3\}$$

$$\cdot [\|\nabla u\|^2 + \|\nabla v\|^2 + \|\nabla w\|^2] + 2\sqrt{2}c_1(D)(\|u\|^2 + \|v\|^2 + \|w\|^2)^{\frac{3}{2}}$$

$$+ 2\sqrt{2}c_1(D)(\|u\|^2 + \|v\|^2 + \|w\|^2)^{\frac{1}{2}}[\|\nabla u\|^2 + \|\nabla v\|^2 + \|\nabla w\|^2].$$

If $\alpha \in (0, 1/3)$ or if (58) holds, choosing $\varepsilon_1 \in \left(\dfrac{2\alpha}{1-\alpha}, 1 + \bar{\mu}\gamma_3\right)$, from (65) one has:

$$(66) \qquad \dot{V} \leq -(\delta_1 - \delta_2 V^{\frac{1}{2}})V - (\delta_3 - \delta_4 V^{\frac{1}{2}})(\|\nabla u\|^2 + \|\nabla v\|^2 + \|\nabla w\|^2).$$

with $\delta_i > 0$, $(i = 1, 2, 3, 4)$ given by

$$(67) \qquad \delta_1 = \min\{k_1, 1, k_2\}, \qquad \delta_2 = \frac{8c_1(D)}{\alpha\sqrt{\alpha}}$$

$$\delta_3 = \min\{\alpha\gamma_1, \gamma_2, \gamma_3\}, \qquad \delta_4 = \frac{4c_1(D)}{\sqrt{\alpha}}.$$

Hence

$$(68) \qquad V(0)^{\frac{1}{2}} < \min\left\{\frac{\delta_1}{\delta_2}, \frac{\delta_3}{\delta_4}\right\},$$

implies, by recursive argument, that $\bar{E}$ is nonlinearly (locally) asymptotically stable with respect to the V-norm

7. STABILITY RESULTS FOR ROBIN BOUNDARY CONDITIONS AND DISCUSSION

In this Section we analyze – via numerical simulations – (2) under Robin boundary conditions

$$(69) \qquad \beta_i X_i + (1 - \beta_i)\nabla X_i \cdot \mathbf{n} = \beta_i \overline{X}_i, \quad \text{on } \partial D \times \mathbb{R}^+, \quad i = 1, 2, 3,$$

with $\beta_i \in (0, 1)$, $\beta_1 = \beta_2 \neq \beta_3$ and $\overline{X}_i$ assigned positive-valued bounded functions $(i = 1, 2, 3)$. In this case $X_i \in H^1(D, \beta_i)$, $(i = 1, 2, 3)$. Let us denote by $\tilde{\mu}_1$ and μ_1 the small eigenvalues of (25) in $H^1(D, \beta_1 = \beta_2)$ and $H^1(D, \beta_3)$ respectively. Concerning the stability analysis of $\bar{E}$, following step by step the procedure used in Section 5, theorems 4–5 continue to hold with $\tilde{\mu}_1$ at the place of μ_2 and μ_1 at the place of σ_2.

In order to explore some specific configurations in the parameters space, that lead to different dynamic behaviors of the system (2), (69) and of the counterpart system of ODEs, let us refer, for the sake of simplicity, to a one-dimensional domain. We provide now some numerical simulations that highlight the relevance of the diffusion action: a steady state stable (unstable) according to the ODEs model, can become unstable (stable) for large sets of values of the diffusion coefficients γ_i $(i = 1, 2, 3)$, which is of great relevance in the study of real phenomena. In fact, as performed in Figure 1, by choosing $\alpha = 1.1$ according to (37), the solution of the counterpart system of ODEs obtained from (2) disregarding the diffusion, reaches the unique constant steady state $\bar{E} \equiv (1, 1.1, 1.1)$, starting from non-zero initial data $X_1^0 = 0.1$, $X_2^0 = 0.03$, $X_3^0 = 0.2$. The behavior of the system,
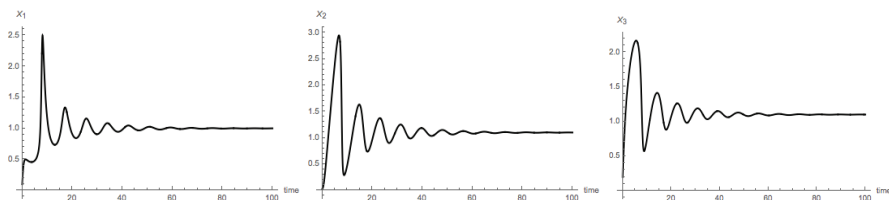
Figure 1. Trajectories of the counterpart system of ODEs when $\alpha = 1.1$ and $X_1^0 = 0.1$, $X_2^0 = 0.03$, $X_3^0 = 0.2$.
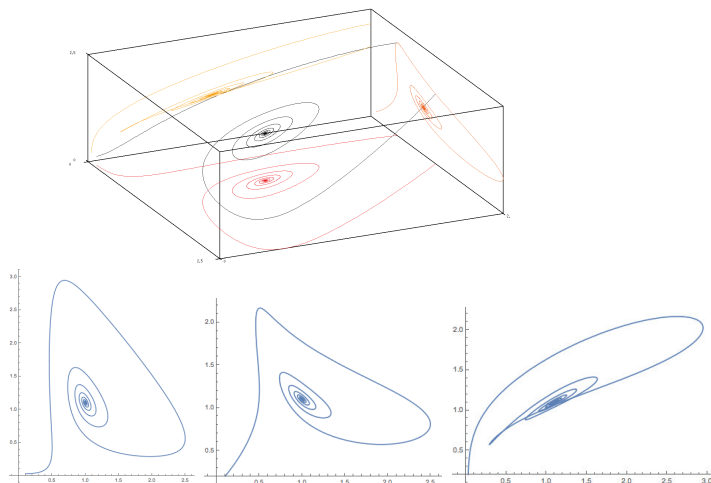

Figure 2. Phase space plot in stable regime: $\alpha = 1.1$, $X_1^0 = 0.1$, $X_2^0 = 0.03$, $X_3^0 = 0.2$. Top: The system approaches the steady state. Bottom: Enlargement of the projections on $X_1 X_2$ plane (left plot), $X_1 X_3$ plane (middle plot), $X_2 X_3$ plane (right plot) of the trajectory near the steady state.

in the stable regime characterized by the same data set as in Figure 1, is painted in the top box of Figure 2. A magnification of the projections on $X_1 X_2$ plane (left plot), $X_1 X_3$ plane (middle plot), $X_2 X_3$ plane (right plot) of the trajectory, near the steady state, has been shown in the bottom plot of Figure 2. For such a value set for α, the trajectories of the system (2), with $\gamma_1 = 0.3$, $\gamma_2 = 3$, $\gamma_3 = 0.2$ satisfying (50) and initial data given by $X_1^0 = 0.93$, $X_2^0 = 1.1$, $X_3^0 = 1.1$, as expected, do not go to the steady state (unstable). Precisely, the simulations show that the trajectories oscillate and these dynamics, for the concentrations X_1 (in the left plot), X_2 (middle plot) and X_3 (right plot) are shown in the Figure 3, which well highlight the destabilizing effect of diffusion.

In order to put in evidence the stabilizing effect of the diffusion, we choose $\alpha = 1.22$. For this value of α the trajectories of the counterpart system of ODEs obtained from (2) disregarding the diffusion, starting from non-zero initial data $X_1^0 = 0.1$, $X_2^0 = 0.3$, $X_3^0 = 0.2$ do not reach the steady state $\bar{E} \equiv (1, 1.22, 1.22)$.
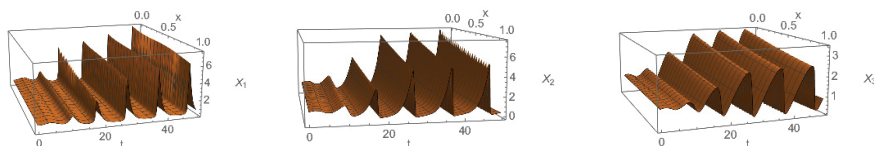
Figure 3. Trajectories of (2) with $\alpha = 1.1$, $\beta_1 = \beta_2 = 0.25$, $\beta_3 = 0.4$, $\gamma_1 = 0.3$, $\gamma_2 = 3$, $\gamma_3 = 0.2$ and $X_1^0 = 0.93$, $X_2^0 = 1.1$, $X_3^0 = 1.1$.
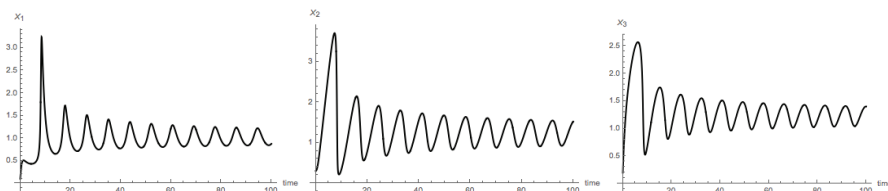

Figure 4. Trajectories of the counterpart system of ODEs with $\alpha = 1.22$, $X_1^0 = 0.1$, $X_2^0 = 0.3$, $X_3^0 = 0.2$.
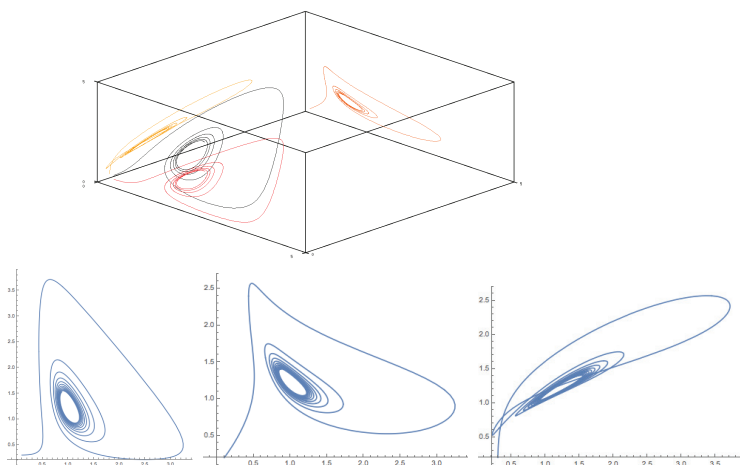

Figure 5. Phase space plot in unstable regime: $\alpha = 1.22$, $X_1^0 = 0.1$, $X_2^0 = 0.3$, $X_3^0 = 0.2$. Top: The system approaches a limit cycle. Bottom: Enlargement of the projections on $X_1 X_2$ plane (left plot), $X_1 X_3$ plane (middle plot), $X_2 X_3$ plane (right plot) of the trajectory, in the vicinity of the limit cycle.

As expected, in this case the equilibrium is unstable. Precisely, for this value of α, according to Remark 1, the system, as performed in Figure 4, shows oscillations, because this value falls into the range characterizing the oscillations. The behavior of system in such unstable regime is well depicted in the top box of Figure 5, where the system approaches a limit cycle. An enlargement of the projections
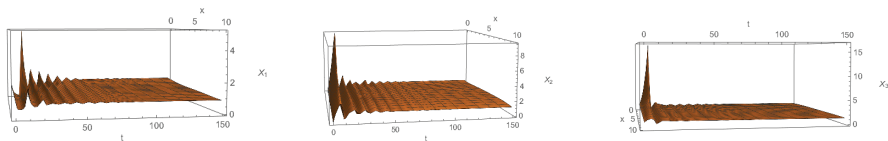
Figure 6. Trajectories of (2) when $\alpha = 1.22$, $\beta_1 = \beta_2 = 0.15$, $\beta_3 = 0.4$, $\mu_1 = 0.5$, $\gamma_1 = 2.2$, $\gamma_2 = 1.5$, $\gamma_3 = 0.5$ and $X_1^0 = 1$, $X_2^0 = 0.005$, $X_3^0 = 1.22$.

on $X_1 X_2$ plane (left plot), $X_1 X_3$ plane (middle plot), $X_2 X_3$ plane (right plot) of the above-mentioned trajectory is given in the bottom plot of Figure 5. The approximate period of a periodic solution when α is near $\alpha_c = (9 - \sqrt{17})/4$ is given by $T_c = 2\pi/\omega \simeq 8.37$, where $\omega \simeq 0.75$ is the approximate angular frequency (pulsation), calculated by (40).

For $\alpha = 1.22$, choosing $\beta_1 = \beta_2 = 0.15$, $\beta_3 = 0.4$ and according to (43), $\gamma_1 = 2.2$, $\gamma_2 = 1.5$, $\gamma_3 = 0.5$, $\mu_1 = 0.5$ the trajectories of the system (2), starting from initial data $X_1^0 = 1$, $X_2^0 = 0.005$, $X_3^0 = 1.22$, as expected, stabilize reaching the equilibrium $\bar{E} = (1, 1.22, 1.22)$.

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