2.2.5 Application of Stability Analysis: The Brusselator

In Chapter 1, we introduced the Brusselator model as the first “chemical” model to demonstrate oscillations and traveling waves. We will now analyze the Brusselator to illustrate how one might use the techniques that we have discussed to establish the behavior of a two-dimensional system. We recall that the equations are:

\[
\begin{align*}
A & \rightarrow X \\
B + X & \rightarrow Y + D \\
2X + Y & \rightarrow 3X \\
X & \rightarrow E
\end{align*}
\]  

(2.60a)  
(2.60b)  
(2.60c)  
(2.60d)

Let the concentrations, like the species, be represented by capital letters, and call the time \( T \). Then, the rate equations for \( X \) and \( Y \) corresponding to eqs. (2.60), with the concentrations of \( A \) and \( B \) held constant, are

\[
\begin{align*}
\frac{dX}{dT} &= k_1 A - k_2 BX + k_3 X^2 Y - k_4 X \\
\frac{dY}{dT} &= k_2 BX - k_3 X^2 Y
\end{align*}
\]  

(2.61a)  
(2.61b)

There are a lot of rate constants floating around in eqs. (2.61). Wouldn’t it be nice if they were all equal to unity? This seems like too much to hope for, but it turns out that if we define a unitless time variable and unitless concentrations, which we shall represent with lower-case letters, then eqs. (2.61) take a much simpler form. We set

\[
X = \alpha x, \quad Y = \beta y, \quad T = \gamma t, \quad A = \delta a, \quad B = \epsilon b
\]  

(2.62)
and substitute eqs. (2.62) into eqs. (2.61) to obtain, after multiplying through by \(\alpha/\gamma\) and \(\alpha/\beta\) in eqs. (2.63a) and (2.63b), respectively,

\[
\frac{dx}{dt} = \left(k_1 \delta \gamma/\alpha\right) a - \left(k_2 \varepsilon \gamma\right) b x + \left(k_3 \alpha \beta \gamma\right) x^2 y - \left(k_4 \gamma\right) x \tag{2.63a}
\]

\[
\frac{dy}{dt} = \left(k_2 \varepsilon \alpha \gamma/\beta\right) b x - \left(k_3 \gamma \alpha^2\right) x^2 y \tag{2.63b}
\]

However, it looks like we have only made things worse, much worse, because eqs. (2.63) contain not only the rate constants but also the scaling factors, \(\alpha, \beta, \gamma, \delta,\) and \(\varepsilon\) that we introduced in eq. (2.62). Now, here comes the trick! We are free to choose the scaling factors any way we like. Let us pick them so as to make all the expressions in parentheses in eqs. (2.63) equal to unity. That is, we shall require that

\[
k_1 \delta \gamma/\alpha = k_2 \varepsilon \gamma = k_3 \alpha \beta \gamma = k_4 \gamma = k_2 \varepsilon \alpha \gamma/\beta = k_3 \gamma \alpha^2 = 1 \tag{2.64}
\]

Equation (2.64) seems to represent six conditions on our five unknown scaling factors, but one condition turns out to be redundant, and a little algebra gives us our solutions:

\[
\alpha = \beta = \left(\frac{k_4}{k_3}\right)^{1/2}, \quad \gamma = 1/k_4, \quad \delta = \left(\frac{k_4}{k_1}\right)\left(\frac{k_4}{k_3}\right)^{1/2} \quad \varepsilon = k_4 k_2 \tag{2.65}
\]

If we now substitute eqs. (2.65) into eqs. (2.63), we obtain a much prettier version of the Brusselator in terms of non-dimensional or unitless variables. This rescaling procedure is often exceedingly useful for reducing the number of parameters (in this case to zero!) before analyzing the properties of a model. We recommend it highly. Our equations are now
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\[
\frac{dx}{dt} = a - bx + x^2y - x \tag{2.66a}
\]
\[
\frac{dy}{dt} = bx - x^2y \tag{2.66b}
\]

To obtain the steady state(s) of the Brusselator, we set eqs. (2.66) equal to zero and solve for \(x\) and \(y\). We find a single solution:

\[
x_{ss} = a, \quad y_{ss} = b/a \tag{2.67}
\]

To analyze the stability of this state, we must calculate the elements of the Jacobian matrix:

\[
J = \begin{bmatrix}
\frac{\partial(dx/dt)}{\partial x} & \frac{\partial(dx/dt)}{\partial y} \\
\frac{\partial(dy/dt)}{\partial x} & \frac{\partial(dy/dt)}{\partial y}
\end{bmatrix} \tag{2.68}
\]
The elements of the Jacobian matrix are

\[
\left. \frac{\partial (dx/dt)}{\partial x} \right|_{ss} = -b + 2a(b/a) - 1 = b - 1 \quad (2.69a)
\]

\[
\left. \frac{\partial (dx/dt)}{\partial y} \right|_{ss} = a^2 \quad (2.69b)
\]

\[
\left. \frac{\partial (dy/dt)}{\partial x} \right|_{ss} = b - 2a(b/a) = -b \quad (2.69c)
\]

\[
\left. \frac{\partial (dy/dt)}{\partial y} \right|_{ss} = -a^2 \quad (2.69d)
\]

We need to obtain the eigenvalues of the matrix whose elements are given by eqs. (2.69) by solving the characteristic equation:

\[
\det \begin{bmatrix} b - 1 - \lambda & a^2 \\ -b & -a^2 - \lambda \end{bmatrix} = 0 \quad (2.70)
\]
or equivalently

\[ \lambda^2 + (a^2 + 1 - b)\lambda + a^2 = 0 \quad (2.71) \]

At this point, although it would not be terribly difficult, we do not need to solve explicitly for \( \lambda \) because we are interested in the qualitative behavior of the system as a function of the parameters \( a \) and \( b \). When a system undergoes a qualitative change in behavior (such as going from a stable steady state to an unstable one) as a parameter is varied, it is said to have undergone a bifurcation. Bifurcations, which we shall discuss further in the next section, occur when the roots of the characteristic equation change sign. A knowledge of the bifurcations of a system is often sufficient to afford a qualitative understanding of its dynamics.

Comparing eqs. (2.57) and (2.71), we observe that \( \text{tr} (J) = -a^2 + b - 1 \), which can be either positive or negative, while \( \det (J) = a^2 \), which is always positive. The stability of the steady state will depend on the sign of the trace. As we vary \( a \) and/or \( b \), when the trace passes through zero, the character of the steady state will change; a bifurcation will occur. If

\[ b > a^2 + 1 \quad (2.72) \]

the sole steady state will be unstable and, thus, by the Poincaré–Bendixson theorem the system must either oscillate or explode. It is possible to prove that the system cannot explode, but is confined to a finite region of the \( x-y \) phase space. Equation (2.72) therefore determines the boundary in the \( a-b \) constraint space between the region where the system will asymptotically approach a stable steady state and the region where it will oscillate periodically.