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Hopf Bifurcation Analysis of Chaotic Chemical Reactor Model

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HOPF BIFURCATION ANALYSIS IN CHAOTIC CHEMICAL REACTOR MODEL

by

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ABSTRACT

Bifurcations in Huang's chaotic chemical reactor system leading from simple dynamics into chaotic regimes are considered. Following the linear stability analysis, the periodic orbit resulting from a Hopf bifurcation of any of the six fixed points is constructed analytically by the method of multiple scales across successively slower time scales, and its stability is then determined by the resulting final secularity condition. Furthermore, we run numerical simulations of our chemical reactor at a particular fixed point of interest, alongside a set of parameter values that forces our system to undergo Hopf bifurcation. These numerical simulations then verify our analysis of the normal form.

TABLE OF CONTENTS

CHAPTER 1: INTRODUCTION

The chaotic chemical reactor model proposed by Huang [1] - [2] is an interesting system to study as it gives rise to a broad range of dynamics. These dynamics stem from the nonlinear components of two autocatalytic steps in the reaction. The governing equations for this reaction are:

$$\begin{aligned} \frac{dx}{dt} &= x(a - px - y - z) \\ \frac{dy}{dt} &= y(x - c) \\ \frac{dz}{dt} &= z(b - x - qz) \end{aligned} \tag{1.1}$$

Since [1] - [2] consider only limited solution classes, we consider the dynamics of this system systematically in this paper.

The system possesses six fixed points. For positive parameters a, b, c, p and q, the only fixed(alternatively, equilibrium or critical) point of (1.1) where each x_0, y_0, z_0 are non-zero is:

$$(x_0, y_0, z_0) = \left(c, \frac{c + aq - b - cpq}{q}, \frac{b - c}{q}\right) \tag{1.2}$$

Chapter 2 considers the basic stability of this fixed point, and the five other ones, as well as their local bifurcations, including those resulting from zero eigenvalues of the Jacobian matrix (transcritical, saddle-node, or pitchfork) as well as regular Hopf and general Hopf bifurcations.

As a path into the next more complex attractors, i.e., limit cycles, we next consider Hopf bifurcations at the fixed points. Following a Hopf bifurcation, one may have one of three possible scenarios:

1. A new stable periodic orbit or attractor created by a supercritical bifurcation, further bifurcations of which may lead into chaotic regimes via the usual period doubling and other routes, or

2. A post-subcritical-bifurcation scenario with no stable local attractors and the system blowing up in finite time (an attractor at infinity), or

3. A different post-subcritical-bifurcation scenario where there are no stable local attractors, but the existence of significant volume reduction can force the system to remain bounded. Strong dissipation often leads to, or is indicative of, a nonlocal attractor, but of course is not a guarantee or proof of it. In this case, the only remaining possibility, other than a global quasiperiodic attractor, is the formation of a nonlocal attractor (via the usual stretching and folding mechanism) on which the system exhibits long-term bounded aperiodic dynamics.

We explore these three possible scenarios by deriving a "normal form" for the periodic orbits appearing after Hopf bifurcation. This "normal form" is derived in Chapter 3, and we use this result to make predictions for the stability of the period orbits in Chapter 4. Finally in Chapter 5, these predictions from the normal form are verified using numerical simulations. Other limit cycles, not resulting from Hopf bifurcations, are also considered there in the large five parameter space for this system.

CHAPTER 2: LINEAR STABILITY

There are several fixed points of this system. In this section we perform linear analysis on the fixed points by examining the system's Jacobian matrix and resulting characteristic polynomial at each fixed point. We present each fixed point in its own subsection. Note that we only consider bifurcations that happen at natural parameter values, i.e. parameter values that are positive and non-zero.

Our linear analysis is explained by the process detailed below. Consider the following system of two ODEs:

$$\dot{x} = f_1(x, y)$$
$$\dot{y} = f_2(x, y)$$

with fixed point x^*, y^* such that $\dot{x} = \dot{y} = 0$. Then if we perturb the fixed point with some $\Delta x, \Delta y$ small enough such that the linearization of the system given by the Jacobian matrix evaluated at x^*, y^* dominates the nonlinearity at this perturbation, then we can find solutions:

$$\dot{\Delta x} = C_1 e^{\lambda_1 t} + C_2 e^{\lambda_2 t}$$
$$\dot{\Delta y} = C_3 e^{\lambda_1 t} + C_4 e^{\lambda_2 t}$$

where C_i is determined by initial conditions of the system, and λ_1, λ_2 are the eigenvalues of the Jacobian matrix at this fixed point. The consequence of this representation for the system at a small perturbation from the fixed point is that the eigenvalues control the growth of $\dot{\Delta x}$, and $\dot{\Delta y}$. We get the following cases depending on what the eigenvalue are:

1. λ_1 and λ_2 are both real and negative. This corresponds to a sink where as $t \to \infty$ we see that Δx and Δy decrease towards zero. This sinking behavior corresponds to a stable node.

2. λ_1 and λ_2 are complex-valued and their real parts are negative. Since they are complex-valued we see from the corresponding trigonometric representation that Δx and Δy will still decay back to the fixed point, but will also feature an oscillatory behavior.

3. λ_1 and λ_2 are positive and real. This results in $\Delta x, \Delta y$ increasing towards ∞ which corresponds to moving away from the fixed point. Since every point near the fixed point gets kicked away, we see that this fixed point is an unstable node.

4. λ_1 and λ_2 are complex-valued and their real parts are positive. Similar to the stable case for complex-conjugate eigenvalues, but instead the oscillatory behavior will be unstable and diverge from the fixed point.

5. λ_1 and λ_2 differ in sign, but are real-valued. In this case as $t \to \infty$ we will have the positive λ term dominate the representation for $\Delta x, \Delta y$. This may occur after significant time depending on the constants C_i and so this behavior is a saddle-node bifurcation.

6. $\lambda_1 = \lambda_2 = 0$ or $\lambda_{1,2} = 0 \pm mi$. This case is special because we cannot make conclusions about the stability of the fixed point by linearization alone. This is because the nonlinear terms which we have ignored control the stability.

This kind of linear analysis can be extended to systems of three dimensions such as ours. The process remains the same, except that we now obtain a third eigenvalue to consider.

Throughout our linear analysis of the chaotic chemical reactor system we will be looking for single, double, and triple-zero bifurcations. These occur when there are $\lambda = 0$ roots of the characteristic polynomial with multiplicity ranging from 1 to 3.

We also search for two types of Hopf bifurcations, the *regular* Hopf bifurcation, where $r_1 \neq 0$ and $r_{2,3}$ are complex conjugates with real part zero, and the *genera*l Hopf bifurcation, where $r_{2,3}$ are complex conjugates with real part zero and $r_1 = 0$. To search for the regular Hopf bifurcation we examine the constants of the characteristic equation in the form:

$$\lambda^3 + b_1\lambda^2 + b_2\lambda + b_3 \tag{2.1}$$

We desire this equation to be factored into the form:

$$(\lambda + r_1)(\lambda^2 + \omega^2) \tag{2.2}$$

where $\omega = |r_2| = |r_3|$. Now by expanding this factored form we get:

$$(\lambda + r_1)(\lambda^2 + \omega^2) = \lambda^3 + r_1\lambda^2 + \omega^2\lambda + r_1\omega^2 \tag{2.3}$$

Therefore $b_1 = r_1$, $b_2 = \omega^2$, and $b_3 = r_1\omega^2$, and so for a regular Hopf bifurcation we must satisfy the necessary condition:

$$b_3 = b_1 b_2 \tag{2.4}$$

Adapting the structure from above in order to find a necessary condition for the general Hopf bifurcation can be done by substituting $r_1 = 0$ which results in the necessary condition:

$$b_1 = 0 \text{ and } b_3 = 0 \tag{2.5}$$

We will use (2.4) and (2.5) at each of the following six fixed points. In addition we find that the non-evaluated Jacobian matrix for our system is:

$$J(x, y, z) = \begin{bmatrix} a - 2px - y - z & -x & -x \\ y & x - c & 0 \\ -z & 0 & b - x - 2qz \end{bmatrix} \tag{2.6}$$

This concludes our introduction to the linear analysis for the system. We now perform the linear analysis at each of the six fixed points to obtain information about bifurcations that occur in our system.

Fixed Point: $\left(0, 0, \frac{b}{q}\right)$

The characteristic polynomial of the Jacobian (2.6) evaluated for this fixed point is:

$$\lambda^3 + \frac{\lambda^2}{q}(b - aq + bq + cq) + \frac{\lambda}{q}(b^2 + bc - abq - acq + bcq) + \frac{1}{q}(b^2c - abcq)$$

We can obtain a single-zero bifurcation by setting $b = aq$, since the constant term will be zero, and we can then factor out the root: $\lambda = 0$. Naturally occurring double and triple-zero bifurcations do not occur, since after substituting in $b = aq$ the characteristic equation becomes:

$$\lambda^3 + c\lambda^2 + aq\lambda^2 + acq\lambda$$

and for the λ^1 term to disappear we would require a, c or q to equal zero.

We also find that this fixed point does not emit any regular or general Hopf bifurcations for naturally occurring parameter values of the system, and so we explore other fixed points.

$$\text{Fixed Point: } \Big(c, c - ap, 0\Big)$$

The characteristic polynomial for this fixed point is:

$$\lambda^3 - \lambda^2(b - c - cp) - \lambda(-ac + bcp) - abc + ac^2 + bc^2p - c^3p$$

For the single-zero bifurcation we can obtain two naturally occurring parameter relations that lead to this type of bifurcation. They are:

$$a = cp$$

$$b = c$$

Their resulting characteristic polynomials are:

$$\lambda^3 + \lambda^2(cp - b + c) + \lambda(c^2p - bcp)$$

$$\lambda^3 + \lambda^2 cp + \lambda(ac - c^2p)$$

If we combine the two parameter relations, that is, our parameters satisfy $a = cp$ and $b = c$, then this will lead into a double-zero bifurcation with the characteristic polynomial $\lambda^3 + \lambda^2 cp$. We see from this that we cannot have a triple-zero bifurcation happening at naturally occurring parameters because either c or p must be zero.

To conclude the linear analysis at this fixed point we observe that the fixed point does not undergo any regular or general Hopf bifurcations.

$$\text{Fixed Point: } \left(\tfrac{a}{p}, 0, 0\right)$$

The characteristic polynomial for this fixed point is:

$$\lambda^3 - \lambda^2(b-a-c) - \frac{\lambda}{p^2}(a^2 - abp - acp + abp^2 - acp^2 + bcp^2) - \frac{1}{p^2}(a^3 - a^2bp - a^2cp + abcp^2)$$

This undergoes a single-zero bifurcation when $a = bp$, which results in the characteristic polynomial $\lambda^3 + \lambda^2(-b + c + bp) + \lambda(-b^2p + bcp)$. We can extend this into a double-zero bifurcation simply by setting $b = c$, yielding the following polynomial $\lambda^3 + \lambda^2 cp$. This cannot undergo a triple-zero bifurcation without c or p being zero.

Finally, this fixed point does not undergo any type of Hopf bifurcation for naturally occurring parameter values, similar to the earlier sections.

$$\text{Fixed Point: } \left(\tfrac{aq-b}{pq-1}, 0, \tfrac{bp-a}{pq-1}\right)$$

The characteristic polynomial for this fixed point is:

$$\frac{1}{(pq-1)^2}\Big(C_1\lambda^3 + C_2\lambda^2 + C_1\lambda + C_4\Big)$$

where the constants C_i are:

$$C_1 = \left(1 - 2pq + p^2q^2\right)$$
$$C_2 = -b + c + bp + 2aq - apq - 2cpq - bp^2q - 2apq^2 + ap^2q^2 + bp^2q^2 + cp^2q^2$$
$$C_3 = -ab + bcp + a^2q - abq + acq + 2abpq + b^2pq - acpq - bcpq - b^2p^2q -$$
$$bcp^2q + a^2q^2 - 2a^2pq^2 - abpq^2 - acpq^2 + abp^2q^2 + acp^2q^2 + bcp^2q^2$$
$$C_4 = ab^2 - abc - b^3p + b^2cp - 2a^2bq + a^2cq + 2ab^2pq - b^2cp^2q + a^3q^2 - a^2bpq^2 - a^2cpq^2 + abcp^2q^2$$

From this characteristic polynomial we can obtain a single-zero bifurcation for the following two parameter relations:

$$a = bp$$
$$a = \frac{b - c + cpq}{q}$$

and their resulting characteristic polynomials are:

$$\lambda^3 - \lambda^2(b - c - bp) - \lambda(b^2p - bcp)$$
$$\lambda^3 + \lambda^2\left(b + c(-1 + p)\right) + \frac{\lambda}{q}\left(c^2(1 - pq) - bc(1 - pq)\right)$$

We see that we can extend the first condition $a = bp$ into a double-zero bifurcation by additionally requiring $b = c$ which yields the polynomial $\lambda^3 - cp\lambda^2$. This polynomial cannot naturally have $\lambda = 0$ as a third root since b or p would have to be zero. Similarly, for the second parameter relation $a = \frac{b-c+cpq}{q}$ we can extend this into a double-zero bifurcation only by setting $b = c$ since we cannot set $pq = 1$ (we would be dividing by zero in the fixed point). This yields the same polynomial after extension as the first parameter relation did.

We now check to see if the fixed point can naturally undergo any Hopf bifurcations. We observe that for the following parameter relations we achieve regular Hopf bifurcations when

$$a = \frac{bp - bpq}{q(p-1)}$$
$$p = \frac{aq}{aq + bq - b}$$

For the first parameter relation if we use the parameter values:

$$b = 20 \quad c = 25 \quad p = \frac{1}{2} \quad q = \frac{3}{2} \quad a = \frac{20}{3}$$

then we obtain the polynomial:

$$\lambda^3 - 15\lambda^2 + 133.333\lambda - 2000$$

which has roots $r_1 = 15, r_{2,3} = \pm 11.547i$.

For the second parameter relation if we use the parameter values:

$$a = 1 \quad b = 10 \quad c = 5 \quad q = 2 \quad p = \frac{1}{6}$$

then we obtain the polynomial:

$$\lambda^3 - 7\lambda^2 + 8\lambda - 56$$

which has roots $r_1 = 7, r_{2,3} = \pm 2\sqrt{2}i$.

We can also find a general Hopf bifurcations happening at this fixed point by adding an additional relation, $c = -\frac{b}{p-1}$ to the first Hopf bifurcation parameter $a = \frac{bp-bpq}{q(p-1)}$. Since we set $p = \frac{1}{2}$ for this relation we will have $c > 0$ to maintain a natural condition, and from $b = 20$ we get that $c = 40$ causes a general Hopf bifurcation to occur. The resulting characteristic polynomial is $\lambda^3 + 133.333\lambda$, with roots $r_1 = 0, r_{2,3} = \pm 11.547i$ as desired.

Origin Fixed Point: $\Big(0, 0, 0\Big)$

The characteristic polynomial resulting from the Jacobian matrix at this fixed point is:

$$\lambda^3 + \lambda^2(c - a - b) + \lambda(ab - ac - bc) + abc$$

Since we do not allow any of our parameters to be zero we cannot have the constant term in our polynomial vanish. As a result we cannot achieve any single, double, or triple-zero bifurcations for this fixed point. Furthermore we cannot achieve a general Hopf bifurcation either as a necessary condition for this type of bifurcation is that the constant term be zero. All that remains is whether a regular Hopf bifurcation can occur.

Observing that the necessary condition for this type of bifurcation requires $b_1 b_2 = b_3$, we get that $b_1 b_2 - b_3 = -(a + b)(a - c)(b - c) = 0$ This can only happen naturally by letting $a = c$ or $b = c$. If we do this our characteristic polynomial becomes either $\lambda^3 - b\lambda^2 + c^2\lambda + bc^2$ or $\lambda^3 - a\lambda^2 - c^2\lambda + ac^2$. In both cases these polynomials will always have real roots, and thus cannot undergo Hopf bifurcations.

Non-Zero Fixed Point: $\left(c, \frac{c+aq-b-cpq}{q}, \frac{b-c}{q}\right)$

The characteristic polynomial of the Jacobian matrix evaluated at this fixed point is:

$$\lambda^3+\lambda^2\left(b+cp-c\right)+\lambda\frac{\left(acq+bcqp-2bc-2c^2(pq-1)\right)}{q}+\frac{abcq-b^2c-ac^2q-c^3(1-pq)-bc^2(pq-2)}{q}$$

We first explore the single, double, and triple-zero bifurcations that can occur at this fixed point. We obtain a single-zero bifurcation when the constant term in this polynomial vanishes. This can occur for the following two parameter relations:

$$a = \frac{b-c+cpq}{q} \tag{2.7}$$

$$b = c \tag{2.8}$$

Their resulting polynomials are:

$$\lambda^3 + \frac{\lambda^2}{q}\left(bq + c(-1+p)q\right) + \frac{\lambda}{q}\left(c^2(1-pq) + bc(-1+pq)\right) \tag{2.9}$$

$$\lambda^3 + c\lambda^2 p + \lambda(ac - c^2 p) \tag{2.10}$$

Now we can extend these two single-zero bifurcations into double-zero bifurcations by using both of the relations together. We see that if $b = c$ then (7) reduces to $a = cp$. Using this in $(9) - (10)$ we get that the b_2 terms in each disappear, yielding a double-zero bifurcation. The resulting characteristic polynomial is:

$$\lambda^3 + cp\lambda^2 \tag{2.11}$$

which cannot give a triple-zero bifurcation at natural points. We could have instead forced a double-zero bifurcation by setting $p = \frac{1}{q}$ since this would kill the b_2 term in (9). If we do this then our resulting polynomial is:

$$\lambda^3 + \frac{\lambda^2}{q}(c + bq - cq) \tag{2.12}$$

We see that if $q = -\frac{c}{b-c}$ which can be positive given $c > b$, that the λ^2 term disappears. Therefore given the parameter values $a = 1, b = 2, c = 4, p = .5, q = 2$, the fixed point undergoes a triple-zero bifurcation.

Following standard methods of phase-plane analysis, we find that the non-zero fixed point undergoes a regular Hopf bifurcation when:

$$q = \frac{(b-c)(b-c+2cp)}{p(b^2 + ac - 2bc + c^2 + bcp - 2c^2p)} \tag{2.13}$$

By setting $a = 30, b = 16.5, c = 10, p = .5$ taken from [2], we get the bifurcating parameter $q = .660508$. The characteristic polynomial at this fixed point is:

$$\lambda^3+\lambda^2(b+cp-c)+\frac{\lambda}{q}\Big(c(aq+c(2-2pq)+b(-2+pq)\Big)-\frac{1}{q}\Big(b-c)c(b-aq+c(-1+pq)\Big) \tag{2.14}$$

After substituting our parameter values and solving for λ we get that the three roots are $r_1 = -11.5, r_{2,3} = \pm 9.25645i$. Since the real part of $\lambda_{2,3}$ is zero this fixed point clearly undergoes a Hopf bifurcation here.

We also get a second possible Hopf bifurcation when:

$$a = \frac{(b-c)(b+c(-1+2p)) - p((b-c)^2 + (b-2c)cp)q}{cpq} \tag{2.15}$$

Using the parameter values $b = 5, c = 6, p = 3, q = .25$ we get the bifurcating parameter $a = 13.0556$. The characteristic polynomial becomes:

$$\lambda^3 + 17\lambda^2 + 0.333333\lambda + 5.66667$$

with roots $r_1 = -17, r_{2,3} = \pm\frac{\sqrt{3}}{3}i$.

We now search for parameter relations that satisfy the general Hopf bifurcation. First we find that when

$$a = -\frac{(b-c)(q-1)}{q} \quad p = -\frac{b-c}{c} \tag{2.16}$$

Then to keep all the parameters positive, we take $b = 10, c = 15, q = 2$ and the two bifurcating parameters $a = 2.5, p = \frac{1}{3}$, which gives the characteristic polynomial $\lambda^3 + 12.5\lambda$. Having as its roots $r_1 = 0, r_{2,3} = \pm 3.53553i$.

We can obtain another general Hopf bifurcation with the parameter relations:

$$b = -\frac{(a(-1+p)q)}{p(-1+q)} \quad c = \frac{aq}{p(-1+q)} \tag{2.17}$$

Keeping all parameters positive we use $a = 5, p = .5, q = 1.5$ and the bifurcating parameters become $b = 15, c = 30$, which yields the characteristic polynomial $\lambda^3 + 75\lambda$. This polynomial has roots $r_1 = 0, r_{2,3} = \pm 8.66025i$ as desired.

CHAPTER 3: MULTIPLE SCALES ANALYSIS

In this section, we will use the method of multiple scales to construct analytical approximations for the periodic orbits arising through the Hopf bifurcation of the fixed points of the Chemical Reactor model (1.1) discussed above. The parameter q will be used as the control parameter. The limit cycle is determined by expanding about the fixed point $(x_0, y_0, z_0) = (10, 15.1591, 9.84091)$ and for the parameters:

$$a = 30, b = 16.5, c = 10, p = .5 \tag{3.1}$$

using progressively slower time scales. The expansions take the form:

$$x = x_0 + \sum_{n=1}^{3} \epsilon^n x_n(T_0, T_1, T_2) \tag{3.2}$$

$$y = y_0 + \sum_{n=1}^{3} \epsilon^n y_n(T_0, T_1, T_2) \tag{3.3}$$

$$z = z_0 + \sum_{n=1}^{3} \epsilon^n z_n(T_0, T_1, T_2) \tag{3.4}$$

where $T_n = \epsilon^n t$ and ϵ is a small positive non-dimensional parameter that is introduced as a bookkeeping device and will be set to unity in the final analysis. Utilizing the chain rule, the time derivative becomes:

$$\frac{d}{dt} = D_0 + \epsilon D_1 + \epsilon^2 D_2 + \epsilon^3 D_3 ..., \tag{3.5}$$

where $D_n = \partial/\partial T_n$. Using the standard expansion for Hopf bifurcations [3] - [4], the bifurcating parameter q, as well as the other parameters are expanded as:

$$\kappa = \kappa_0 + \epsilon^2 \kappa_2 \tag{3.6}$$

where $q_0 = .660508$ as discussed above. This allows the influence from the nonlinear terms and the control parameter to occur at the same order.

Using (3.2) - (3.6) in (1.1) and equating like powers of ϵ yields equations at O(ϵ^i), $i = 1, 2, 3$ of the form:

$$L_1(x_i, y_i, z_i) = S_{i,1} \tag{3.7}$$

$$L_2(x_i, y_i, z_i) = S_{i,2} \tag{3.8}$$

$$L_3(x_i, y_i, z_i) = S_{i,3} \tag{3.9}$$

where the $L_i, i = 1, 2, 3$ are the differential operators:

$$L_1(x_i, y_i, z_i) = -10a_i + 100p_i + 5x_i + 10y_i + 10z_i + D_0 x_i \tag{3.10}$$

$$L_2(x_i, y_i, z_i) = 15.1591c_i - 15.1591x_i + D_0 y_i \tag{3.11}$$

$$L_3(x_i, y_i, z_i) = -9.84091b_i + 96.8435q_i + 9.84091x_i + 6.5z_i + D_0 z_i \tag{3.12}$$

The source terms $S_{i,j}$ for $i = 1, 2, 3$ and $j = 1, 2, 3$ i.e. at $\mathrm{O}(\epsilon), \mathrm{O}(\epsilon^2)$, and $\mathrm{O}(\epsilon^3)$ are given as follows:

$$
\begin{aligned}
S_{1,1} &= 0 \\
S_{1,2} &= 0 \\
S_{1,3} &= 0 \\
S_{2,1} &= 10a_2 - 100p_2 + a_1x_1 - 20p_1x_1 - 0.5x_1^2 - x_1y_1 - x_1z_1 - D_1x_1 \\
S_{2,2} &= -15.1591c_2 - c_1y_1 + x_1y_1 - D_1y_1 \\
S_{2,3} &= 9.84091b_2 - 96.8435q_2 + b_1z_1 - 19.6818q_1z_1 - x_1z_1 - 0.660508z_1^2 - D_1z_1 \\
S_{3,1} &= 10a_2 - 100p_2 + a_1x_1 - 20p_1x_1 - 0.5x_1^2 - x_1y_1 - x1z1 - D_2x_1 - D_1x_2 \\
S_{3,2} &= -15.1591c_3 - c_2y_1 + x_2y_1 - c_1y_2 + x_1y_2 - D_2y_1 - D_1y_2 \\
S_{3,3} &= 9.84091b_3 - 96.8435q_3 + b_2z_1 - 19.6818q_2z_1 - x_2z_1 - q_1z_1^2 + b_1z_2- \\
&\quad 19.6818q_1z_2 - x_1z_2 - 1.32102z_1z_2 - D_2z_1 - D_1z_2
\end{aligned}
\tag{3.13}
$$

We now find a composite operator that acts on (3.7) - (3.9) at each order. The benefit is that this composite operator will be a function of one variable, and will be used to build the remaining two variables at each order. To do this we note that (3.9) may be solved for x_i in terms of z_i. Using this and solving (3.7) for y_i in terms of (x_i, z_i) allows us to have y_i in terms of z_i only. Finally we can create a composite equation of the three sources by substituting our expressions for x_i and now y_i (both in terms of z_i) into (3.8):

$$L_c z_i = \Gamma_i \tag{3.14}$$

where

$$L_c = -10.0127 + 1.75289D_0 + .726559D_0^2 + .0101617D_0^3 \tag{3.15}$$

and the composite source Γ_i is:

$$\Gamma_i = 1.54042 S_{i3} - S_{i2} + .1 D_0 S_{i1} - .660508 D_0 S_{i3} - .0101617 D_0^2 S_{i3} \tag{3.16}$$

We shall use (3.14) later to identify and suppress secular terms in the solutions of (3.7) - (3.9).

Let us now turn to finding the solutions of (3.7) - (3.9). We will solve order by order using the method of undetermined coefficients, and using these solutions to build the next order. For $i = 1$ or $O(\epsilon)$ we know that the solutions will recreate the linear analysis and so $S_{1,1} = S_{1,2} = S_{1,3} = 0$. Hence we pick up a solution for the first order population using the known eigenvalues (from the previous section) at Hopf bifurcation, i.e.

$$z_1 = e^{i\omega t}\alpha(T_1, T_2) + e^{-i\omega t}\beta(T_1, T_2) + \gamma e^{\lambda_3 t} \tag{3.17}$$

where $\lambda_1 = i\omega = 9.25645i$, and $\beta(T_1, T_2)$ is the complex conjugate of $\alpha(T_1, T_2)$ since λ_2 and λ_1 are complex conjugates of each other. Finally, since z_1 is real, the α and β modes correspond to the center manifold where $\lambda_{1,2}$ are purely imaginary and where the Hopf bifurcation occurs, while γ corresponds to the attractive direction or the stable manifold. Since we wish to construct and analyze the stability of the periodic orbits which lie in the center manifold, we suppress the solution with non-zero real part, i.e., we set:

$$\gamma = 0 \tag{3.18}$$

Using (3.17) and (3.18) in (3.14) - (3.16) for $i = 1$ gives $y_1(T_0, T_1, T_2)$ and $x_1(T_0, T_1, T_2)$:

$$y_1 = C_y e^{-9.25645iT_0}\alpha(T_1, T_2) + \overline{C_y} e^{9.25645iT_0}\beta(T_1, T_2) \tag{3.19}$$

$$x_1 = C_x e^{-9.25645iT_0}\alpha(T_1, T_2) + \overline{C_x} e^{9.25645iT_0}\beta(T_1, T_2) \tag{3.20}$$

Where $C_x = 2.42263 - 6.72536i$ and $C_y = -0.660508 + 0.940609i$.

Now that the first order solutions (3.17), (3.19), and (3.20) are known, the second-order sources $S_{2,1}, S_{2,2}, S_{2,3}$ may be evaluated, using (3.13).

We note that the first order solutions reappear in the second-order source. Therefore the method of undetermined coefficients calls for the second-order solutions (z_2, x_2, y_2) to include the first order multiplied by a factor t. This will cause our approximation to breakdown when this variable t is comparable to ϵ, and so we must suppress these first-order terms for our approximation to be uniformly valid. We call the terms that solve the first-order *secular*.

Setting the coefficients of the secular $e^{\lambda_{1,2}t}$ terms in these sources to zero yields:

$$\frac{\partial \alpha}{\partial T_1} = 0 \qquad \frac{\partial \beta}{\partial T_1} = 0 \tag{3.21}$$

Next, using the second-order sources, and (3.21), the second-order particular solution is taken in the usual form to balance the zeroth and second harmonic terms at this order, i.e.,

$$z_2 = z_{20} + z_{22} e^{2i\omega t} \tag{3.22}$$

Using this in (3.14) for $i = 2$, and balancing the DC, or time-independent, and second-harmonic terms, the coefficients z_{20} and z_{22} in the second-order particular solution (3.22) are found to be:

$$z_{22} = (0.0217567 - 0.019425i)\beta(T_1, T_2)^2 \tag{3.23}$$

$$z_{20} = 14.898919162198q_2 - 1.5832004304\alpha(T_1, T_2, T_3)\beta(T_1, T_2, T_3) \tag{3.24}$$

Using z_2 in (3.7) - (3.9) for $i = 2$, together with the second-order sources, yields the other second-order fields x_2, and y_2. Using these, together with the first-order results, we may evaluate the coefficients of the secular terms in the third-order composite source Γ_3, from (3.13) and (3.14). Suppressing these secular, first-harmonic, terms to obtain uniform expansions yields the final equation for the evolution of the coefficients in the linear solutions on the slow second-order time scales:

$$\frac{\partial \alpha}{\partial T_2} = C_1\alpha + C_2\beta\alpha^2 \tag{3.25}$$

where

$$C_1 = -(32.4796 - 461.182i)q_2 \tag{3.26}$$

$$C_2 = -(4.23697 + 20.3082i) \tag{3.27}$$

This equation (3.25) is the normal form, or simplified system in the center-manifold, in the vicinity of the Hopf bifurcation point(s). We shall now proceed to compare the predictions for the post-bifurcation dynamics from this normal form with actual numerical simulations. In addition, complex solutions in the post-bifurcation regime will be characterized via the use of numerical diagnostics.

CHAPTER 4: NORMAL FORM PREDICTIONS

To proceed, we represent the normal form (3.25) as:

$$\frac{\partial \alpha}{\partial T_2} = (C_{1r} + iC_{1i})\alpha + (C_{2r} + iC_{2i})\beta\alpha^2 \tag{4.1}$$

Writing $\alpha = \frac{1}{2}Ae^{i\theta}$ and separating this equation into real and imaginary parts yields:

$$\frac{\partial A}{\partial T_2} = C_{2r}A^3/4 + C_{1r}A \tag{4.2}$$

$$\frac{\partial \theta}{\partial T_2} = C_{2i}A^2/4 + C_{1i} \tag{4.3}$$

In the usual way, the fixed points of (4.2) give the amplitude of the solution $\alpha = \frac{1}{2}Ae^{i\theta}$. These fixed points are:

$$A_1 = 0, A_{2,3} = \pm\sqrt{-4C_{1r}/C_{2r}} \tag{4.4}$$

with $A_{2,3}$ corresponding to the bifurcating periodic orbits in the post-Hopf regime (as seen by putting $\alpha = \frac{1}{2}Ae^{i\theta}$ in the first-order fields in Equations (3.17), (3.19), and (3.20)). Since $C_{1r} = -32.4796q_2$ and $C_{2r} = -4.23697$, the $A_{2,3}$ are real fixed points (corresponding to real bifurcating periodic orbits) for $q_2 < 0$. Hence, by (3.6), the periodic orbits exist below the Hopf bifurcation value q_0. The Jacobian of (4.2) evaluated at $A_{2,3}$ is $-2C_{1r} = 64.9592q_2 < 0$, thus indicating that these fixed points (the periodic orbits) are stable, and so we can settle on the periodic orbits in the post-Hopf regime. Thus, the Hopf bifurcation at q_0 is *supercritical.* We shall verify this prediction numerically in the next section, and then explore the region of q values below the Hopf bifurcation systematically.

CHAPTER 5: NUMERICAL SIMULATIONS

By approximating the flow of the system in a computer model, we can easily analyze the behavior of the system as parameters are further varied beyond the Hopf bifurcation. Furthermore, by computing the power spectrum of either the x, y, or z values of the flow, we can better understand the bifurcations that are observed, particularly with regards to the period doubling bifurcations, as well as the systems approach to chaos. For this exercise, we have used the initial conditions $x(0) = 0.8, y(0) = 0.5$, and $z(0) = 0.8$ which lie close to, but not on, many of the paths created by the bifurcations.

Figures 5.1 and 5.2 show the limit cycle at $q = 0.66$, just below the Hopf bifurcation value $q = 0.660508$ derived above for the non-zero fixed point $(x_0, y_0, z_0) = (10, 15.1591, 9.84091)$ corresponding to the other parameters taking the values $a = 30, b = 16.5, c = 10, p = .5$.

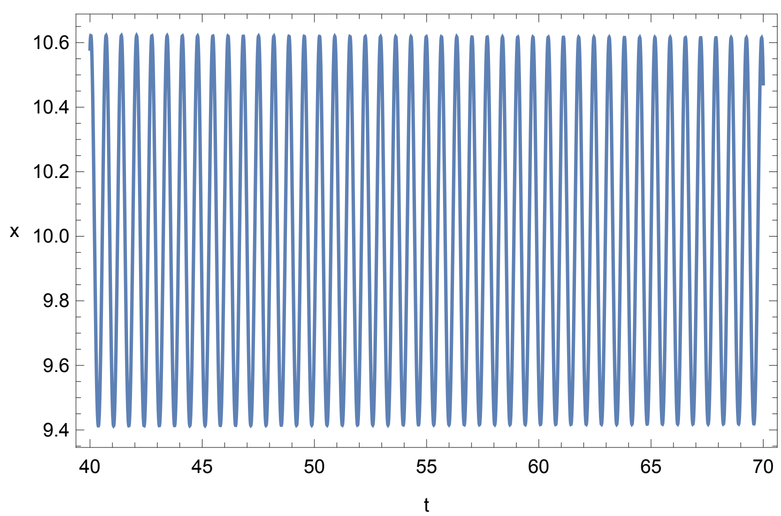

Figure 5.1: Stable Limit Cycle in $x(t)$ close to q_0.

As predicted at the end of the previous section from the use of the normal form, stable limit cycles should be seen below the Hopf bifurcation value of q, since the bifurcation is supercritical, and figure 5.1 indeed shows a periodic solution for $x(t)$.

Figure 5.2 shows the limit cycle in the (x, y, z) phase space and the approach from the initial conditions. Right before the next major bifurcation.

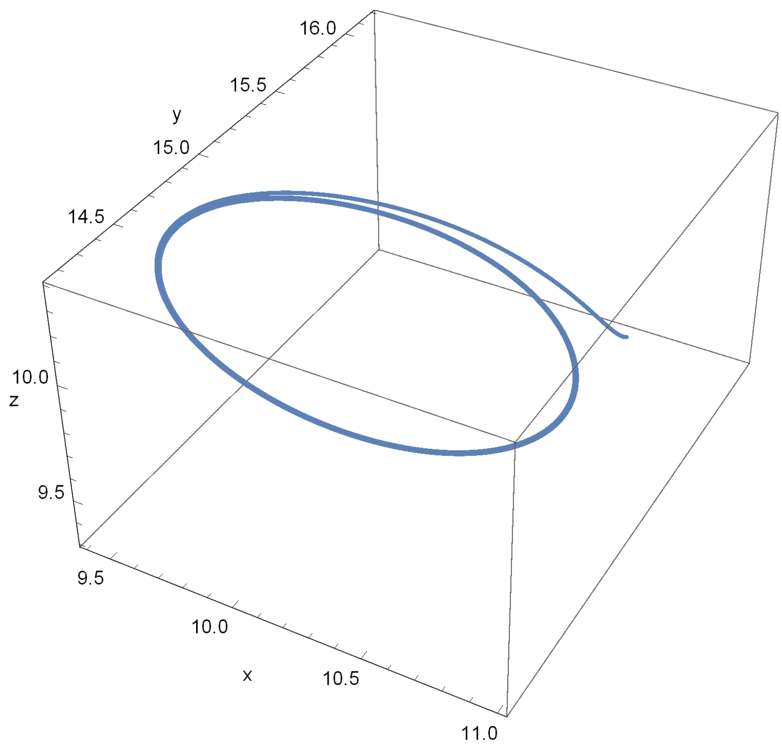

Figure 5.2: The attractor in (x, y, z) phase-space for the parameter set (3.1).

Decreasing the q value very slightly to 0.659, the corresponding solutions for $z(t)$ in figure 5.3 and the (x, y, z) plot of figure 5.6 already show intermittent behavior, and 'fattening' of the phase-space attractor due to further bifurcation of the periodic orbit created by the supercritical Hopf bifurcation. It is straightforward to fine-tune carefully, decreasing q in very small steps to track these bifurcations, using a combination of phase-space plots and power spectral density diagnostics, or Floquet multiplier calculations, to classify this bifurcation of the primary Hopf-created periodic orbit as period doubling, symmetry-breaking, or a secondary Hopf bifurcation [5].

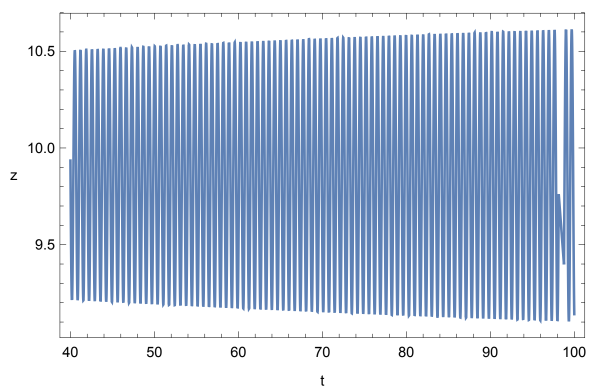

Figure 5.3: The limit cycle slowly unwinds since we moved away from q_0.

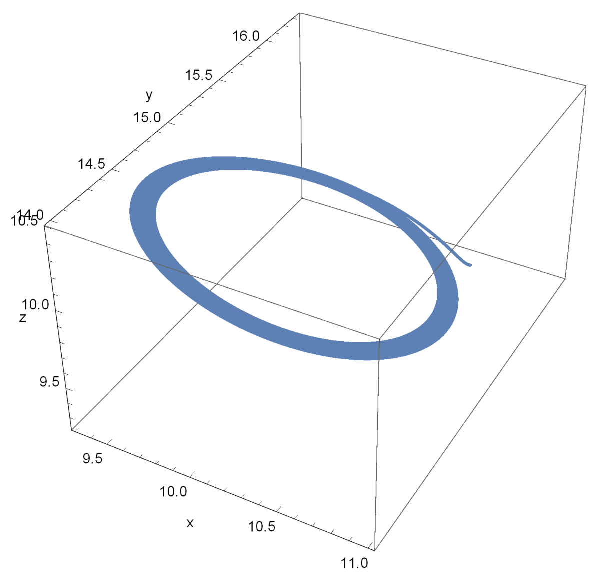

Figure 5.4: The limit cycle that is being warped by desultory behavior of the system.

With so many parameters in our chemical model, stable limit cycles may of course occur in many other regions of the large multiparameter space, and not even necessarily near a point of Hopf bifurcation. Figures 5.5 and 5.6 shows such a stable periodic orbit for the parameter set $a = 40, b = 20, c = 14, p = 0.4, q = 0.4$. This particular limit cycle is quite robust, unlike the Hopf-created one discussed above, and persists over the entire range of p values $(0.2, 1.25)$ if the other parameters are kept unchanged.

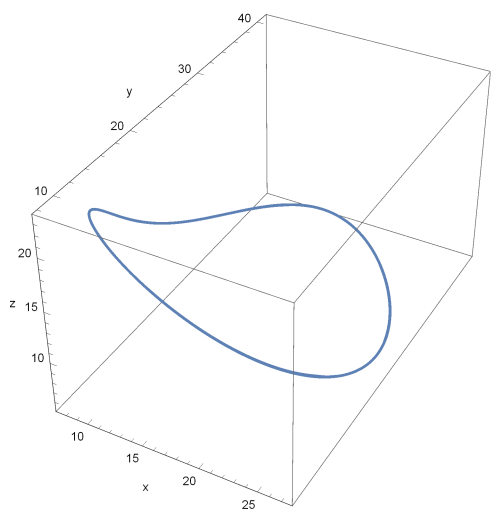

Figure 5.5: Stable limit cycle occurring far away from the Hopf bifurcation.

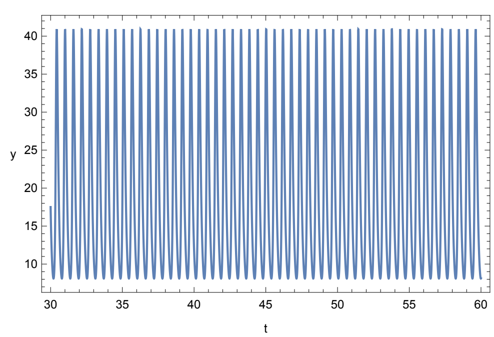

Figure 5.6: The stable limit cycle from above displayed in $y(t)$.

Searching for more complex dynamics beyond periodic solutions in a model like (1.1) with a large number of parameters is virtually like looking for a needle in a haystack since there are many routes depending on which parameter or set of parameters is varied. Our analysis enables this search to be far more refined, and we hope that further research into the dynamics past the point of Hopf bifurcation will be considered.

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