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Two-parameter periodic solutions near a Hopf point in delay-differential equations

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Abstract. Time delays can occur naturally or as transport lags in many physico-chemical as well as biological systems. Incorporating them into a lumped parameter system results in a system of first-order ordinary delay-differential equations (DDEs). In this paper, we develop two-parameter periodic solutions near a Hopf point in such systems using the general reductive perturbation theory and apply the results to a nonisothermal chemical reactor with delayed feedback. The paper suggests that the two-parameter result can be generalized to multiple time delays and other parameters. Results of this work can be useful in constructing plane wave solutions, rotating waves, phase singularity and other interesting phenomena for temporal kinetic systems with time delays.

1. Introduction

Analysis of dynamical systems in the presence of time delays has been a topic of interest to researchers in diverse fields. The time delays appear as the intrinsic or extrinsic character of a system. These time delays can alter the stability characteristics of the dynamics. For example, the transport of reactant species from one site to another before the reaction takes place in Goodwin's model (MacDonald 1973) describing protein synthesis and cell metabolism is an example of an intrinsic time lag. On the other hand, a reactor designed for a low conversion reaction may have a recycle of the unreacted material from the reactor products. This recycle feedback will experience a transport lag, which is an example of an extrinsic time delay. Such delays also occur in other reactors such as spark engines with intrinsic time delays and plug flow reactors with delayed recycles (Schell and Ross 1986). Recently, Inamdar and Kulkarni (1993) analysed the kinetic instabilities in reaction–diffusion systems for an exponential autocatalytic reaction. For the same system, Inamdar *et al* (1991) studied the onset of kinetic and diffusive instabilities in the absence of a time delay and the stability of plane wave solutions. These plane wave solutions, which are uniform oscillations, lie very close to the Hopf point. Such an analysis for the delay-differential equations (DDEs) will indeed be useful in studying the effect of time delays on chemical instabilities. An equation of small amplitude motion will help in further investigation into higher-order transitions. It will also help in knowing whether the kinetic or the diffusive effects will cause an instability first in a reaction dynamics. Thus the analysis will be a key result in the design of various types of chemical and biological reactors. This is our motivation for further research on systems with time delays.

Feedbacks in many open non-equilibrium systems such as autocatalysis, cross-catalysis, etc and other types of feedback loops are responsible for complex nonlinear behaviour in such

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systems. For instance, many chemical reaction systems, when far from equilibrium, show exotic bifurcation patterns leading to multi-stationarity and/or periodic or quasi-periodic or even chaotic oscillations. An intrinsic or extrinsic time lag present in a system can give rise to a more complex spatio-temporal organization of open non-equilibrium systems. In many biochemical systems, intrinsic time delays arise due to the transport of chemical species across a membrane or the transmission of a signal by circulating hormones or the regulation of reaction pathways etc. MacDonald (1978) gives an excellent summary of biological systems having discrete and distributed time lags. Analyses of these systems have shown that the time delay can destabilize a stationary state resulting in periodic oscillations. Several investigations also suggest that time delays can be responsible for biochemical oscillations. For instance, Rapp (1974) showed that biochemical oscillations arise due to end product inhibition with a time delay. Mackey and Glass (1977) reported an onset of respiratory disorders, while Buchholtz and Schneider (1987) simulated DNA replication in T3/T7 bacteriophage in the presence of time delays.

Schell and Ross (1986) detailed the effect of time lags on the temporal evolution of homogeneous chemical reactions and also on trajectories near the saddle and periodic orbits. They also showed the presence, due to time delay, of chaos and hyperchaos near these bifurcation points. Roesky *et al* (1993) experimentally studied the *B-Z* reaction with a built-in time delay between the input and the output to the reacting system and observed a variety of periodic states by changing the time delay and coupling strengths. Even chaotic states were observed which were not seen during the delay-free running of the oscillator for the same residence time. Inamdar *et al* (1991) studied the effect of time delay on a non-isothermal continuously stirred tank reaction (CSTR) with a first-order exothermic reaction. They found that time delay can lead to a torus-like formation in a phase plane for a stable limit cycle of a CSTR dynamics without delay. They also reported the formation of kinks and knots for limit cycle solutions in a three-solution region for various sets of parameters.

In this study, we consider the effect of simultaneous perturbations in a system parameter and a time delay. We first give a two-dimensional motivating example of a non-isothermal continuous stirred tank reactor with a recycle. Through this example, we illustrate the main steps of the procedure in this paper. Then, we present the full analysis for a general system of DDEs. In that, we first derive the evolution equations with perturbations in the two parameters and then derive a non-trivial periodic solution for a small amplitude orbital motion near a Hopf point. Finally, we reconsider the motivating example and illustrate the application of our general result by performing all numerical calculations for a Hopf point in the example system.

2. Motivating example

For illustrating the main steps of our general derivation, we consider a non-isothermal chemical reactor (CSTR) with a time-delayed feedback recycle. Its dynamics are described (Uppal *et al* 1974) by the following DDEs:

$$\begin{aligned}\frac{dX}{dt} &= -X + \gamma e^Y(1 - X) + (1 - R)X(t - \tau) \\ \frac{dY}{dt} &= -Y + \mu \gamma e^Y(1 - X) - \alpha Y + (1 - R)Y(t - \tau)\end{aligned}$$

and its stationary solutions are given by the implicit equations $\exp[Y_s] = RX_s / [\mu(1 - X_s)]$ and $X_s = (\alpha + R)Y_s / (\mu R)$. First, we define deviational state variables $\mathbf{x}(t) = (X(t) - X_s, Y(t) - Y_s)^T$ and $\mathbf{y}(t) = \mathbf{x}(t - \tau)$ and express the right-hand side of the above DDEs as a

Taylor series in x and y about the stationary state to get,

$$\frac{dx}{dt} = Ax + By + Cxx + Dxy + Eyy + Fxxx + Gxxy + Hxyy + Pyyy + \dots \quad (1)$$

where the various matrices are given by,

$$\begin{aligned} A &= \begin{pmatrix} -1 - \gamma e^{Y_s} & \gamma(1 - X)e^{Y_s} \\ -\mu\gamma e^{Y_s} & -(1 + \alpha) + \mu\gamma(1 - X_s)e^{Y_s} \end{pmatrix} \\ B &= (1 - R)I \\ C &= \frac{\gamma e^{Y_s}}{2} \begin{pmatrix} 0 & -1 & -1 & 1 - X_s \\ 0 & -\mu & -\mu & \mu(1 - X_s) \end{pmatrix} \\ D &= E = G = H = P = \mathbf{0} \\ F &= \frac{\gamma e^{Y_s}}{6} \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & -1 & -1 & 1 - X_s \\ 0 & 0 & 0 & -\mu & 0 & -\mu & -\mu & \mu(1 - X_s) \end{pmatrix} \end{aligned}$$

and xx , xy , etc are Kronecker products $x \otimes x$, $x \otimes y$, and so on.

In addition to the delay τ , the above system has four possible parameters γ , α , μ , and R . Each parameter by itself may lead to oscillations in this system beyond a critical value. However, it may happen that a combination of two parameters also results in oscillations. Our interest in the above system is to examine the combined effect of two parameters μ and τ near a Hopf point. We assume that $(\mu = \eta, \tau = \beta)$ is a critical combination representing a Hopf point. In this section, we perform a perturbation analysis near this point using the reductive perturbation theory to obtain equations describing system oscillations. To this end, we first define two perturbation parameters ϵ and δ by $\mu = \eta + \chi_1\epsilon^2$ and $\tau = \beta + \chi_2\delta^2$, where $\chi_1 = \text{sgn}(\mu - \eta)$ and $\chi_2 = \text{sgn}(\tau - \beta)$.

The main idea behind our approach is to express all terms in equation (1) as series expansions in ϵ and δ to derive perturbation equations. Then we solve these equations to get an expression for the system oscillations characterized by a pair of purely imaginary eigenvalues. Thus, we postulate a solution,

$$\begin{aligned} x(t) &= \epsilon x_{10} + \delta x_{01} + \epsilon^2 x_{20} + 2\epsilon\delta x_{11} + \delta^2 x_{02} + \epsilon^3 x_{30} + 3\epsilon^2\delta x_{21} + \dots \\ y(t) &= \epsilon x_{10}(t - \tau) + \delta x_{01}(t - \tau) + \epsilon^2 x_{20}(t - \tau) + 2\epsilon\delta x_{11}(t - \tau) + \dots \end{aligned}$$

Since $t - \tau = t - \beta - \chi_2\delta^2$, we expand $x_{ij}(t - \tau)$ as a Taylor series about $t - \beta$ to get,

$$x_{ij}(t - \tau) = y_{ij}(t) - \chi_2\delta^2 \frac{\partial y_{ij}(t)}{\partial t} + \frac{\delta^4}{2} \frac{\partial^2 y_{ij}(t)}{\partial t^2} - \dots$$

where, $y_{ij}(t) = x_{ij}(t - \beta)$. The above equation can be substituted in the earlier expression for $y(t)$ to get an expansion of $y(t)$ in terms of $y_{ij}(t)$.

We seek a solution in terms of various timescales t , $\theta_{10} = \epsilon t$, $\theta_{01} = \delta t$, $\theta_{20} = \epsilon^2 t$, $\theta_{02} = \delta^2 t$, etc. To this end, we express the total time derivative in terms of the timescales using the chain rule of differentiation as,

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \epsilon \frac{\partial}{\partial \theta_{10}} + \delta \frac{\partial}{\partial \theta_{01}} + \epsilon^2 \frac{\partial}{\partial \theta_{20}} + \epsilon\delta \frac{\partial}{\partial \theta_{11}} + \delta^2 \frac{\partial}{\partial \theta_{02}} + \dots$$

Finally, since A , C , F etc are also functions of μ , we expand them as Taylor series about $\mu = \eta$ to get,

$$\begin{aligned} A &= A_0 + \chi_1\epsilon^2 A_1 + \epsilon^4 A_2 + \dots \\ A_0 &= A(\mu = \eta) \\ A_1 &= \gamma e^{Y_s} \begin{pmatrix} 0 & 0 \\ -1 & 1 - X_s \end{pmatrix} \\ A_2 &= A_3 = A_4 = A_5 = \dots = \mathbf{0}. \end{aligned}$$

Having expanded all of the terms in the DDEs as series in ϵ and δ , we substitute them back into the DDEs and compare the coefficients of various orders of ϵ and δ from both sides of the DDEs. Since this can be done easily using a symbolic manipulation software and it is pointless to give all the details, we give the resulting equations for only the first-order terms, i.e. those involving ϵ and δ , as follows:

$$\begin{aligned}\frac{\partial x_{10}}{\partial t} - A_0 x_{10} - B_0 y_{10} &= 0 \\ \frac{\partial x_{01}}{\partial t} - A_0 x_{01} - B_0 y_{01} &= 0.\end{aligned}$$

The next step is to solve the above differential equations and the others from higher orders to get expressions $x_{ij}(t)$, but we stop here. Having illustrated the basic idea behind our procedure through this example, we proceed directly to address a general system of DDEs. At the end of this paper, we will apply our results to this example system and present numerical results.

3. Perturbation analysis

Let a general autonomous system with one time delay be described by the following DDEs:

$$\begin{aligned}\dot{X}(t) &= \Gamma[X(t), Y(t), \mu] & X(0) &= X_0 & X, Y &\in \mathbf{R}^n \\ Y(t) &= X(t - \tau)\end{aligned}\quad (2)$$

where μ is a system parameter, $\tau > 0$ is a time delay, and \mathbf{R}^n is an n -dimensional Euclidean space. Let $X(t) = X_s$ be a stationary solution for the above system. Clearly $Y(t) = X_s$ at steady state. Then equation (2) in its local (deviational) form becomes,

$$\dot{x} = f(x, y, \mu) \quad x, y \in \mathbf{R}^n \quad (3)$$

where $x(t) = X(t) - X_s$ and $y(t) = Y(t) - X_s$.

In the extreme cases of $\tau = 0$ and $\tau = \infty$, μ is the only bifurcation parameter of interest. A finite τ , which can affect system stability and bifurcation patterns, becomes a second parameter in the above system. Thus, perturbations in μ and τ , either individually or jointly, can cause oscillations in the system and a two-parameter study is warranted to account for both parameters simultaneously.

Let a critical combination ($\mu = \eta, \tau = \beta$) represent a Hopf bifurcation point in equation (3). We analyse the system behaviour in the neighbourhood of this critical point arising due to perturbations in μ and τ . Furthermore, we are interested in perturbations that destabilize the system into periodic oscillations. In other words, we assume that there exists a pair of eigenvalues with zero real parts for the linearized system at this Hopf point and all other eigenvalues have negative real parts, so that any perturbation in parameters makes the system oscillate. We wish to derive a single two-parameter equation describing such small amplitude oscillatory motion of the system. As done in example (1), we define two perturbation parameters ϵ and δ by $\mu = \eta + \chi_1 \epsilon^2$ and $\tau = \beta + \chi_2 \delta^2$, where $\chi_1 = \text{sgn}(\mu - \eta)$ and $\chi_2 = \text{sgn}(\tau - \beta)$.

For using the method of multiple timescales, we define the perturbation timescales $\theta_{ij} = \epsilon^i \delta^j t$, $i = 0, \infty, j = 0, \infty$, thus $\theta_{00} = t$ is the fast timescale and the rest are the slow timescales. In other words, now $t \equiv t(\theta_{ij})$ and $x(t) \equiv x(\epsilon, \delta, \theta_{ij})$. As mentioned earlier, our strategy will be to write perturbation expansions for the various components of equation (3) to expand both its (left and right) sides as perturbation series in terms of $\epsilon^i \delta^j$. Equating the series coefficients from both sides will give us a series of perturbation equations which will describe the system motion in different timescales.

Thus, we start with the expansions of $x(t)$ and $y(t)$. We assume the following two-parameter expansion for x :

$$x(\epsilon, \delta) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{(i+j)!}{i!j!} \epsilon^i \delta^j x_{ij}(\theta_{ij}) \quad x_{00} = 0. \quad (4)$$

Using the above, $y(t)$ becomes

$$y(t) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{(i+j)!}{i!j!} \epsilon^i \delta^j x_{ij}(t - \tau). \quad (5)$$

Since $t - \tau = t - \beta - \chi_2 \delta^2$, each $x_{ij}(t - \tau)$ can be further expanded as a Taylor series about $(t - \beta)$ as

$$x_{ij}(t - \tau) = y_{ij}(t) + \sum_{k=1}^{\infty} \frac{(-\chi_2)^k}{k!} \delta^{2k} \frac{\partial^k y_{ij}(t)}{\partial t^k}$$

$$y_{ij}(t) = x_{ij}(t - \beta).$$

Using the above in equation (5), rearranging the series and renaming the indices, we get

$$y(\epsilon, \delta) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \epsilon^i \delta^j \left[y_{ij} + \sum_{k=1}^{[j/2]} \frac{(i+j-2k)! (-\chi_2)^k}{i!(j-2k)!k!} \frac{\partial^k y_{i(j-2k)}}{\partial t^k} \right] \quad (6)$$

where $y_{00} = 0$ and $[j/2]$ denotes the greatest integer less or equal to $j/2$.

Let us now expand the time-derivative operator $\Theta \equiv d/dt$. We define operators $\Theta_{ij} = \partial/\partial\theta_{ij}$ and express Θ using the chain rule as

$$\Theta(\epsilon, \delta) = \Theta_{00} + \epsilon \Theta_{10} + \delta \Theta_{01} + \epsilon^2 \Theta_{20} + \epsilon \delta \Theta_{11} + \delta^2 \Theta_{02} + \dots \quad (7)$$

From equations (4) and (7), the right-hand side Θx of equation (3) also becomes a perturbation series. We define the coefficients of this series by the following:

$$\Theta(\epsilon, \delta)x(\epsilon, \delta) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{(i+j)!}{i!j!} \epsilon^i \delta^j g_{ij}. \quad (8)$$

Finally, we expand $f(x, y)$ as a Taylor series about the stationary state,

$$f(x, y) = Ax + By + Cxx + Dxy + Eyy + Fxxx + Gaxy + Hxyy + Pyyy + \dots$$

where the partial differential operators A, B , etc are $A = f_x$, $B = f_y$, $C = f_{xx}/2!$, $D = f_{xy}$, $E = f_{yy}/2!$, $F = f_{xxx}/3!$, $G = f_{xxy}/2!$, $H = f_{xyy}/2!$ and $P = f_{yyy}/3!$, where f_{xy} denotes $\partial^2 f/\partial x \partial y$, etc. Since these operators are all functions of μ only, we further expand them as Taylor series about $\mu = \eta$. Using $\mu(\epsilon) = \eta + \chi_1 \epsilon^2$, we get,

$$A = \sum_{i=0}^{\infty} (\chi_1)^i \epsilon^{2i} A_i \quad (9)$$

$$B = \sum_{i=0}^{\infty} (\chi_1)^i \epsilon^{2i} B_i \quad (10)$$

$$A_i = \frac{1}{i!} \left[\frac{\partial^{i+1} f}{\partial x \partial \mu^i} \right]_{\epsilon=\delta=0} \quad B_i = \frac{1}{i!} \left[\frac{\partial^{i+1} f}{\partial y \partial \mu^i} \right]_{\epsilon=\delta=0} \dots$$

With the help of above operators, the right side of equation (3) also becomes a perturbation series in ϵ and δ . Analogous to equation (8), we define the coefficients of this series by

$$f(\epsilon, \delta) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{(i+j)!}{i!j!} \epsilon^i \delta^j f_{ij}. \quad (11)$$

Comparing the coefficients of expansions of $\Theta \mathbf{x} = \mathbf{f}$ (equation (3)) in equations (8) and (11), we get $\mathbf{g}_{ij} = \mathbf{f}_{ij}$, $i = 0, \infty$, $j = 0, \infty$, as the series of perturbation equations. These perturbation equations are nothing but partial differential equations describing the system motion. In the next section, we evaluate the \mathbf{f}_{ij} and \mathbf{g}_{ij} to identify these differential equations.

4. Perturbation equations

Since derivation of the \mathbf{g}_{ij} and the \mathbf{f}_{ij} involves tedious algebra, we start with the first-order ($i + j = 1$) terms and then proceed step by step up to the third-order terms. Since terms up to the third order suffice to fully describe the small amplitude motion (i.e. the motion in first order), we do not consider the higher-order terms. We evaluate \mathbf{g}_{ij} and \mathbf{f}_{ij} by using a symbolic manipulator. Note that $\mathbf{g}_{00} = 0$. For the first-order ($i + j = 1$) coefficients, we get, $\mathbf{g}_{ij} = \Theta_{00}\mathbf{x}_{ij}$, $\mathbf{f}_{ij} = \mathbf{A}_0\mathbf{x}_{ij} + \mathbf{B}_0\mathbf{y}_{ij}$ and the first-order perturbation equations ($\mathbf{g}_{ij} = \mathbf{f}_{ij}$ for $i + j = 1$) are,

$$(\Theta_{00} - \mathbf{A}_0)\mathbf{x}_{ij} - \mathbf{B}_0\mathbf{y}_{ij} = 0 \quad (i + j = 1). \quad (12)$$

These are the two fundamental homogeneous equations for the system. They imply $\mathbf{x}_{10} = \mathbf{x}_{01} \equiv \mathbf{x}_1$ and $\mathbf{y}_{10} = \mathbf{y}_{01} \equiv \mathbf{y}_1$.

Using the above simplifications in evaluating the second-order ($i + j = 2$) coefficients, we get, $\mathbf{g}_{20} = \Theta_{00}\mathbf{x}_{20} + \Theta_{10}\mathbf{x}_1$, $\mathbf{g}_{11} = \Theta_{00}\mathbf{x}_{11} + (\Theta_{10} + \Theta_{01})\mathbf{x}_1/2$, $\mathbf{g}_{02} = \Theta_{00}\mathbf{x}_{02} + \Theta_{01}\mathbf{x}_1$, and $\mathbf{f}_{ij} = \mathbf{A}_0\mathbf{x}_{ij} + \mathbf{B}_0\mathbf{y}_{ij} + \mathbf{C}_0\mathbf{x}_1^2 + \mathbf{D}_0\mathbf{x}_1\mathbf{y}_1 + \mathbf{E}_0\mathbf{y}_1^2$. Therefore, the perturbation equations ($\mathbf{g}_{ij} = \mathbf{f}_{ij}$, $i + j = 2$) become,

$$\begin{aligned} (\Theta_{00} - \mathbf{A}_0)\mathbf{x}_{20} - \mathbf{B}_0\mathbf{y}_{20} &= \mathbf{C}_0\mathbf{x}_1^2 + \mathbf{D}_0\mathbf{x}_1\mathbf{y}_1 + \mathbf{E}_0\mathbf{y}_1^2 - \Theta_{10}\mathbf{x}_1 \\ (\Theta_{00} - \mathbf{A}_0)\mathbf{x}_{11} - \mathbf{B}_0\mathbf{y}_{11} &= \mathbf{C}_0\mathbf{x}_1^2 + \mathbf{D}_0\mathbf{x}_1\mathbf{y}_1 + \mathbf{E}_0\mathbf{y}_1^2 - (\Theta_{10} + \Theta_{01})\mathbf{x}_1/2 \\ (\Theta_{00} - \mathbf{A}_0)\mathbf{x}_{02} - \mathbf{B}_0\mathbf{y}_{02} &= \mathbf{C}_0\mathbf{x}_1^2 + \mathbf{D}_0\mathbf{x}_1\mathbf{y}_1 + \mathbf{E}_0\mathbf{y}_1^2 - \Theta_{01}\mathbf{x}_1. \end{aligned} \quad (13)$$

For the above three equations to have a periodic solution, a condition known as the solvability condition (Kuramoto 1984) or the Fredholm alternative (Iooss and Joseph 1990) must be satisfied. Applying the solvability condition to the above equations, we get $\Theta_{10}\mathbf{x}_1 = \Theta_{01}\mathbf{x}_1 = 0$. With this result, the above three equations reduce to one equation and we define $\mathbf{x}_2 = \mathbf{x}_{ij}$ and $\mathbf{y}_2 = \mathbf{y}_{ij}$ for $i + j = 2$.

Similarly, evaluating the third-order ($i + j = 3$) coefficients, we get the following third-order perturbation equations:

$$\begin{aligned} (\Theta_{00} - \mathbf{A}_0)\mathbf{x}_{30} - \mathbf{B}_0\mathbf{y}_{30} &= \mathbf{h} + [\chi_1(\mathbf{A}_1\mathbf{x}_1 + \mathbf{B}_1\mathbf{y}_1) - \Theta_{20}\mathbf{x}_1] \\ (\Theta_{00} - \mathbf{A}_0)\mathbf{x}_{21} - \mathbf{B}_0\mathbf{y}_{21} &= \mathbf{h} + [\chi_1(\mathbf{A}_1\mathbf{x}_1 + \mathbf{B}_1\mathbf{y}_1) - \Theta_{20}\mathbf{x}_1 - \Theta_{11}\mathbf{x}_1]/3 \\ (\Theta_{00} - \mathbf{A}_0)\mathbf{x}_{12} - \mathbf{B}_0\mathbf{y}_{12} &= \mathbf{h} - [\chi_2\mathbf{B}_0\Theta_{00}\mathbf{y}_1 - \Theta_{02}\mathbf{x}_1 - \Theta_{11}\mathbf{x}_1]/3 \\ (\Theta_{00} - \mathbf{A}_0)\mathbf{x}_{03} - \mathbf{B}_0\mathbf{y}_{03} &= \mathbf{h} - [\chi_2\mathbf{B}_0\Theta_{00}\mathbf{y}_1 - \Theta_{02}\mathbf{x}_1] \end{aligned} \quad (14)$$

where, $\mathbf{h} = \mathbf{F}_0\mathbf{x}_1^3 + \mathbf{G}_0\mathbf{x}_1^2\mathbf{y}_1 + \mathbf{H}_0\mathbf{x}_1\mathbf{y}_1^2 + \mathbf{P}_0\mathbf{y}_1^3 + 2\mathbf{C}_0\mathbf{x}_1\mathbf{x}_2 + \mathbf{D}_0(\mathbf{x}_1\mathbf{y}_2 + \mathbf{x}_2\mathbf{y}_1) + 2\mathbf{E}_0\mathbf{y}_1\mathbf{y}_2$.

Before we derive the solutions for the various \mathbf{x}_{ij} ($1 \leq i + j \leq 3$), we first analyse the two-parameter perturbation expansion of the eigenvalue problem for the linearized system. This is needed because the \mathbf{x}_{ij} will be expressed in terms of its eigenvalues and eigenvectors.

4.1. Eigenvalue problem

The eigenvalue problem for the linearized equation (3) is,

$$(\mathbf{A} + e^{-\lambda\tau}\mathbf{B})\mathbf{U} = \lambda\mathbf{U} \quad (15)$$

and the characteristic polynomial is,

$$\det[A + e^{-\lambda\tau} B - \lambda I] = 0$$

where U is the right unit eigenvector. We now expand both the eigenvalues and the eigenvector U in the neighbourhood of this two-parameter critical point. Since both are perturbation functions of μ and τ , we expand them as Taylor series around $(\epsilon = 0, \delta = 0)$ to obtain,

$$\lambda = \lambda_0 + \chi_1 \lambda_{20} \epsilon^2 + \chi_2 \lambda_{02} \delta^2 + \lambda_{40} \epsilon^4 + \chi_1 \chi_2 \lambda_{22} \epsilon^2 \delta^2 + \lambda_{04} \delta^4 + \dots \quad (16)$$

$$U = U_0 + \chi_1 \epsilon^2 U_{20} + \chi_2 \delta^2 U_{02} + \dots \quad (17)$$

Using equation (16) and $\tau = \beta + \chi_2 \delta^2$, we obtain,

$$e^{-\lambda\tau} = e^{-\lambda_0\beta} [1 - \chi_1 \beta \lambda_{20} \epsilon^2 - \chi_2 (\lambda_0 + \beta \lambda_{02}) \delta^2 + \dots].$$

Now we substitute the above perturbation expansion and those from equations (9), (10), (16) and (17) into equation (15). Then, we collect and compare the coefficients of ϵ^2 and δ^2 order terms on both sides to get

$$(L_0 - \lambda_0)U_0 = 0$$

$$(L_0 - \lambda_0)U_{20} + (A_1 + e^{-\lambda_0\beta} B_1)U_0 = \lambda_{20}(I + \beta e^{-\lambda_0\beta} B_0)U_0$$

$$(L_0 - \lambda_0)U_{02} - \lambda_0 e^{-\lambda_0\beta} B_0 U_0 = \lambda_{02}(I + \beta e^{-\lambda_0\beta} B_0)U_0$$

$$L_0 = A_0 + e^{-\lambda_0\beta} B_0.$$

Let U_0^* be an adjoint eigenvector of U_0 such that $U_0^* L_0 = \lambda_0 U_0^*$, $U_0^* U_0 = 1$ and $U_0^* \bar{U}_0 = 0$. Multiplying both sides of the above equations by U_0^* and simplifying, we get the following results:

$$\begin{aligned} \lambda_0 &= a_0 + b_0 e^{-\lambda_0\beta} \\ \lambda_{20} &= (1 + \beta b_0 e^{-\lambda_0\beta})^{-1} (a_1 + b_1 e^{-\lambda_0\beta}) \\ \lambda_{02} &= (1 + \beta b_0 e^{-\lambda_0\beta})^{-1} (-\lambda_0 b_0 e^{-\lambda_0\beta}) \end{aligned} \quad (18)$$

where $a_0 = U_0^* A_0 U_0$, $b_0 = U_0^* B_0 U_0$, $a_1 = U_0^* A_1 U_0$, and $b_1 = U_0^* B_1 U_0$.

Since our interest is the scenario in which any perturbation in the system parameters causes oscillatory motion, the linearized system must have purely imaginary eigenvalues at the Hopf point. In other words, $\lambda_0 = \pm i\omega_0$, where ω_0 , as we see later, is the fundamental frequency of oscillations in the fast timescale. From here on, we will derive results for $\lambda_0 = i\omega_0$ only. Substituting $\lambda_0 = i\omega_0$ in equation (18), we get,

$$z = e^{-i\omega_0\beta} = \frac{i\omega_0 - a_0}{b_0}.$$

Separating the real and imaginary parts in the above, we get the following explicit expression for ω_0 :

$$\omega_0 = \text{Im } a_0 \pm \sqrt{\|b_0\|^2 - (\text{Re } a_0)^2} \quad (19)$$

where $\text{Re } a_0$ and $\text{Im } a_0$ denote, respectively, the real and imaginary parts of a_0 . Since we must have real positive ω_0 , further analysis of equation (19) reveals that a necessary condition for the oscillatory motion is $\|b_0\| > |\text{Re } a_0|$. Furthermore, $\omega_0 > 0$ is possible only if (a) $\|a_0\| < \|b_0\|$ or (b) $\text{Im } a_0 > 0$ and $\|a_0\| > \|b_0\|$. Note that a unique $\omega_0 > 0$ exists in case (a), while two distinct $\omega_0 > 0$ exist in case (b). However, no solution is possible when $\text{Im } a_0 < 0$ and $\|a_0\| > \|b_0\|$, as $\omega_0 < 0$.

Substituting for ω_0 in equation (18) and solving for β , we get,

$$\beta = \frac{1}{\omega_0} \arctan \left(\frac{\text{Im } b_0 + \Delta \text{Re } b_0}{\text{Re } b_0 - \Delta \text{Im } b_0} \right)$$

where $\Delta = \sqrt{[\|b_0\|^2/(\operatorname{Re} a_0)^2] - 1}$ and $\beta > 0$. Clearly, multiple positive β are possible for a system. The above expression for β gives us a relation between η and β , which must be satisfied for the oscillatory motion at a Hopf point. In other words, it gives us a locus of Hopf bifurcation points for various system parameter values η and β .

5. Equation of motion

We now solve the PDE's (equations (12)–(14)) derived in the previous section. From equations (12), we have,

$$(\Theta_{00} - A_0)x_1 - B_0y_1 = 0.$$

Since we proved earlier that $\Theta_{10}x_1 = \Theta_{01}x_1 = 0$, we assume the following neutral solution for the above equation:

$$x_1(t) = W(\theta_{20}, \theta_{11}, \theta_{02})e^{+i\omega_0 t}U_0 + \bar{W}(\theta_{20}, \theta_{11}, \theta_{02})e^{-i\omega_0 t}\bar{U}_0 \quad (20)$$

where W is a complex field and \bar{W} is its complex conjugate.

From equations (13), we have,

$$(\Theta_{00} - A_0)x_2 - B_0y_2 = C_0x_1^2 + D_0x_1y_1 + E_0y_1^2.$$

Since the inhomogeneous term in the above has only the zeroth and the second-order harmonics after substitution of the assumed neutral solution, we assume the following form of solution for the above equation:

$$x_2(t) = W^2e^{+2i\omega_0 t}V + \bar{W}^2e^{-2i\omega_0 t}\bar{V} + \|W\|^2V_0 + v_0x_1$$

where \bar{V} is the complex conjugate of V . Substituting the above in the previous ordinary differential equation (ODE) and equating terms from both sides gives us

$$\begin{aligned} V &= (2i\omega_0 I - A_0 - zB_0)^{-1}(C_0 + zD_0 + z^2E_0)U_0U_0 \\ \bar{V} &= -(2i\omega_0 I + A_0 + z^{-1}B_0)^{-1}(C_0 + z^{-1}D_0 + z^{-2}E_0)\bar{U}_0\bar{U}_0 \\ V_0 &= -(A_0 + B_0)^{-1}[2C_0 + (z + z^{-1})D_0 + 2E_0]U_0\bar{U}_0 \end{aligned}$$

and v_0 remains undetermined.

We now consider equations (14). Since the inhomogeneous terms in these equations have first-order harmonics, the solvability condition must be satisfied. Substituting for x_1 and x_2 into their inhomogeneous terms and applying the solvability condition, we get the following four Stuart–Landau (SL) equations:

$$\Theta_{20}W = p\|W\|^2W + \chi_1(a_1 + zb_1)W \quad (21)$$

$$\Theta_{20}W + \Theta_{11}W = 3p\|W\|^2W + \chi_1(a_1 + zb_1)W \quad (22)$$

$$\Theta_{02}W + \Theta_{11}W = 3p\|W\|^2W - \chi_2(i\omega_0zb_0)W \quad (23)$$

$$\Theta_{02}W = p\|W\|^2W - \chi_2(i\omega_0zb_0)W \quad (24)$$

$$\begin{aligned} p &= U_0^*[2C_0 + (z^2 + z^{-1})D_0 + 2zE_0]V\bar{U}_0 + U_0^*[2C_0 + (1 + z)D_0 + 2zE_0]U_0V_0 \\ &\quad + U_0^*[3F_0 + (2z + z^{-1})G_0 + (2 + z^2)H_0 + 3zP_0]U_0U_0\bar{U}_0. \end{aligned}$$

From equations (21) and (22), we get,

$$\Theta_{11}W = 2p\|W\|^2W. \quad (25)$$

Thus, a non-trivial solution of the three independent SL equations (equations (21), (24) and (25)) will give us W , which will fully specify the equation of small-amplitude orbital motion. To this end, let the complex amplitude W be expressed in a polar form as:

$$W(\theta_{20}, \theta_{11}, \theta_{02}) = R(\theta_{20}, \theta_{11}, \theta_{02})e^{i\phi_{20}(\theta_{20})}e^{i\phi_{11}(\theta_{11})}e^{i\phi_{02}(\theta_{02})} \quad (26)$$

where R , ϕ_{20} , ϕ_{11} and ϕ_{02} are all real. We define $\sigma_1 + i\omega_1 = a_1 + zb_1$, $\sigma_2 + i\omega_2 = -i\omega_0zb_0$ and $p = p_1 + ip_2$. Substituting W from equation (26) into equations (21), (24) and (25) and separating the real and imaginary parts, we get the following amplitude and phase equations:

$$\Theta_{20}R = \chi_1\sigma_1R + p_1R^3 \quad (27)$$

$$\Theta_{11}R = 2p_1R^3 \quad (28)$$

$$\Theta_{02}R = \chi_2\sigma_2R + p_1R^3 \quad (29)$$

$$\frac{d\phi_{20}}{d\theta_{20}} = \chi_1\omega_1 + p_2R^2 \quad (30)$$

$$\frac{d\phi_{11}}{d\theta_{11}} = 2p_2R^2 \quad (31)$$

$$\frac{d\phi_{02}}{d\theta_{02}} = \chi_2\omega_2 + p_2R^2. \quad (32)$$

Since the amplitude must be constant at steady state, $\Theta R = 0$ at steady state, i.e.

$$\lim_{t \rightarrow \infty} \Theta R = \lim_{t \rightarrow \infty} (\epsilon^2 \Theta_{20} + \epsilon \delta \Theta_{11} + \delta^2 \Theta_{02}) R = 0.$$

Substituting from equations (27)–(29) into the above condition, we get the following expression for the steady-state amplitude R_s :

$$R_s = \frac{1}{\epsilon + \delta} \sqrt{\frac{\chi_1\sigma_1}{-p_1}\epsilon^2 + \frac{\chi_2\sigma_2}{-p_1}\delta^2}.$$

Clearly the argument of the above root must be positive for periodic motion to exist. Setting R to R_s in equations (30)–(32), we derive the phase component solutions at steady state as,

$$\phi_{20} = (\chi_1\omega_1 + p_2R_s^2)\theta_{20}$$

$$\phi_{11} = 2p_2R_s^2\theta_{11}$$

$$\phi_{02} = (\chi_2\omega_2 + p_2R_s^2)\theta_{02}.$$

With these, an approximate solution describing the small amplitude orbital motion becomes,

$$\begin{aligned} \mathbf{X}(t) &\approx \mathbf{X}_s + (\epsilon + \delta)\mathbf{x}_1(t) \\ &= \mathbf{X}_s + \sqrt{\frac{\chi_1\sigma_1}{-p_1}\epsilon^2 + \frac{\chi_2\sigma_2}{-p_1}\delta^2} [e^{i(\omega_0 + \chi_1\omega_{20}\epsilon^2 + \chi_2\omega_{02}\delta^2)t} \mathbf{U}_0 + \text{c.c.}] \\ \omega_{20} &= \omega_1 - \sigma_1 p_2 / p_1 \\ \omega_{02} &= \omega_2 - \sigma_2 p_2 / p_1 \end{aligned}$$

where c.c. stands for the complex conjugate of the preceding term in the bracket. As expected, setting either perturbation parameter to zero, we get the one-parameter result for the other parameter. It is interesting to note that the above two-parameter solution is a simple superposition of the amplitudes and the phases of the constituent one-parameter results. Therefore, a generalization to systems with multiple delays and/or multiple system parameters appears to be obvious.

For the linear stability analysis, we use equations (27)–(29) to get,

$$\frac{dR}{dt} = (\chi_1\sigma_1\epsilon^2 + \chi_2\sigma_2\delta^2)R + p_1(\epsilon + \delta)^2R^3.$$

Linearizing the above about $R = R_s$, we find that the amplitude is linearly stable if $\chi_1\sigma_1\epsilon^2 + \chi_2\sigma_2\delta^2 > 0$, otherwise not. Since p_1 and $(\chi_1\sigma_1\epsilon^2 + \chi_2\sigma_2\delta^2)$ must have opposite signs for a periodic motion to exist, the solution stability is governed by $\text{sgn}(p_1)$. The orbital motion is stable if $p_1 < 0$ and unstable otherwise.

6. Example results

We now reconsider the motivating example described earlier (equation (1)). We will apply the general results from the last section to compute a two-parameter Hopf point in this system and also the corresponding equation of motion. We assume that $\gamma = 0.09$, $\alpha = 3$, $\mu = 30$ and $R = 0.3$. For this set of parameter values, we numerically solve the equation

$$X_s = \frac{R + \alpha}{\mu R} \ln \left[\frac{RX_s}{\gamma(1 - X_s)} \right]$$

to get the stationary state as ($X_s = 0.6183$, $Y_s = 1.6862$) and also to compute the various system matrices A_0 , B_0 , etc as

$$A_0 = \begin{pmatrix} -1.486 & 0.186 \\ -14.577 & 1.564 \end{pmatrix}$$

$$A_1 = \begin{pmatrix} 0 & 0 \\ -0.486 & 0.185 \end{pmatrix}$$

$$B_0 = 0.7I$$

$$C_0 = \begin{pmatrix} 0 & -0.243 & -0.243 & 0.093 \\ 0 & -7.289 & -7.289 & 2.782 \end{pmatrix}$$

$$F_0 = \begin{pmatrix} 0 & 0 & 0 & -0.081 & 0 & -0.081 & -0.081 & 0.031 \\ 0 & 0 & 0 & -2.430 & 0 & -2.430 & -2.430 & 0.927 \end{pmatrix}$$

$$B_1 = D_0 = E_0 = G_0 = H_0 = P_0 = 0.$$

Using the above, the expressions for V , V_0 and p simplify as

$$V = (2i\omega_0 I - A_0 - zB_0)^{-1} C_0 U_0 U_0 \quad (33)$$

$$V_0 = -2(A_0 + B_0)^{-1} C_0 U_0 \bar{U}_0 \quad (34)$$

$$p = 2U_0^* C_0 (V \bar{U}_0 + U_0 V_0) + 3U_0^* F_0 U_0 U_0 \bar{U}_0. \quad (35)$$

To obtain the eigenvectors, we rewrite the characteristic polynomial $\det[A_0 + e^{-i\omega_0\beta} B_0 - i\omega_0 I] = 0$ as $\det[A_0 + \psi I] = 0$ with $\psi = e^{-i\omega_0\beta}(1 - R) - i\omega_0$. Clearly for ω_0 to be real, ψ must be complex. Thus if we define $\psi = \psi_1 + i\psi_2$ and solve the characteristic polynomial we get

$$\psi_1 = -\frac{T}{2} = -0.0393 \quad (T = \text{Trace}[A_0])$$

$$\psi_2 = \pm\sqrt{4D - T^2} = \pm 0.6145 \quad (D = \det[A_0]).$$

Now we solve the eigenvector equations $[A_0 + \psi I]U = U^*[A_0 + \psi I] = \mathbf{0}$ with $\psi = 0.0393 + 0.6145i$ to get U and U^* . We normalize them to get U_0 and U_0^* as follows:

$$U_0 = U/\|U\| = (0.1121 \quad 0.9217 - 0.3714i)^T$$

$$U_0^* = U^*/(U^* \cdot U) = (4.4607 - 11.0714i \quad 1.3464i).$$

Using the above, we calculate $a_0 = U_0^* A_0 U_0$, $b_0 = U_0^* B_0 U_0$ and $b_1 = U_0^* A_1 U_0$ to get $\text{Re } a_0 = 0.0393$, $\text{Im } a_0 = -0.6145$, $\text{Re } b_0 = 0.7$, $\text{Im } b_0 = 0$, $\sigma_1 = \text{Re } b_1 = 0.0927$, and $\omega_1 = \text{Im } b_1 = 0.1569$. Using equation (19), we get one positive root $\omega_0 = 0.0844$. This is the fundamental frequency of oscillations for this example system. Using this, we calculate $z = (i\omega_0 - a_0)b_0 = -0.0561 + 0.9984i$ and using $\psi_1 = (1 - R) \cos \omega_0\beta = -0.0393$, we get $\beta = 1.627$. Thus, $\eta = 30$ and $\beta = 1.627$ constitute a two-parameter Hopf point for this non-isothermal CSTR. Furthermore, we get $\sigma_2 = \text{Re}[-i\omega_0 b_0 z] = 0.059$ and $\omega_2 = \text{Im}[-i\omega_0 b_0 z] = 0.0033$.

Now we are ready to calculate p . To this end, we first obtain $V = (0.4231 - 1.8955i - 2.0233 - 16.5626i)^T$ from equation (33) and $V_0 = (0.2955 \ 0.8059)^T$ from equation (34). Finally, substituting the vectors and matrices into equation (35), we get $p_1 = \text{Re } p = 40.0668$ and $p_2 = \text{Im } p = 4.2961$. Finally, the orbital motion is given by,

$$\mathbf{X}(t) \approx \mathbf{X}_s + 10^{-2} \sqrt{-23.1\chi_1\epsilon^2 - 14.7\chi_2\delta^2} [e^{i(\omega_0 + \chi_1\omega_{20}\epsilon^2 + \chi_2\omega_{02}\delta^2)t} \mathbf{U}_0 + \text{c.c.}]$$

where, $\omega_0 = 0.0844$, $\omega_{20} = 0.147$ and $\omega_{02} = -0.0033$. Since p_1 is positive, the orbital motion is unstable.

7. Conclusion

We used reductive perturbation theory to derive a two-parameter equation for small amplitude orbital motion near a Hopf point in an autonomous system of DDEs with one time delay and one system parameter. The equation of motion indicates that the phases and amplitudes corresponding to the one-parameter motions simply superpose to yield the two-parameter result. Therefore, the final result is easily generalized to a system with two or more time delays and/or system parameters. We also derived a two-parameter locus of Hopf points. We find that several time delays may result into Hopf points for a given system parameter and that two oscillatory solution frequencies may be possible under some conditions at a given Hopf point.

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