PI = performance index
Q = reactant flow rate, cu. ft./sec.
Q_c = cooling water flow rate, cu. ft./sec.
R = gas constant, B.t.u./(lb.-mole)(°R.)
s = Laplace transform variable
T = temperature, °F. or °R.
t = time
U = overall heat transfer coefficient, B.t.u./(sec.)(sq. ft.)(°R.)
V = volume, cu. ft.
W = process parameters excluding adjustable controller parameters

Greek Letters

ρ = density, lb./cu. ft.
τ = time
w = frequency

Subscripts

C = concentration
C = controller
c = cooling water
i = inlet
i = index
j = index
o = initial value
p = process
Sp = signal preceding adjustable parameter in control loop
ss = steady state
set = set point
T = temperature

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Manuscript received September 22, 1967; revision received August 25, 1969; paper accepted September 8, 1969.

Parameter Sensitivity of Systems Described by Nonlinear Ordinary Differential Equations

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An approximate analytical method is developed to estimate the parameter sensitivity of the solution of a set of nonlinear ordinary differential equations describing a system which exhibits periodic behavior. An approximate solution is constructed in terms of both the approximate periodic solution determined from Galerkin equations and the envelope and phase of the oscillation away from such a periodic solution. Parameter sensitivity information is then obtained by examining the parameter variation effect on the approximate solution.

Examples of two- and three-dimensional nonlinear systems illustrate this procedure and show that the effect of parameter change on the solution is predicted with sufficient accuracy to make this method useful for nonlinear analysis.

The behavior of an engineering system under normal operating conditions is influenced by parameter disturbances. If an analytical solution to the set of nonlinear ordinary differential equations describing such a system were available, the effect of parameter changes could be determined in a straightforward manner. However, it is usually difficult or impossible to obtain an analytical solution to nonlinear differential equations. This difficulty has motivated the use of approximations for the analysis of a nonlinear system. Linearization of the set of differential equations is valuable, but it frequently fails to describe the system behavior in a region not very far from the singular point about which the linearization is performed. Fur-

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thermore, linearization gives no information about the size of a stability region or the existence of limit cycles, the knowledge of which is important in engineering design. Linearization combined with the numerical integration of the set of nonlinear differential equations has been successfully employed (*1*, *35*) but could become rather tedious in the investigation of the effects of parameter changes. To overcome the restrictions of this linear analysis followed by numerical integration, nonlinear behavior has been investigated by quasilinear techniques in which the nonlinearities are considered "small" (*4*, *10*, *17*, *23*, *25* to *28*, *38*). These techniques, however, have limitations in analyzing a highly nonlinear system of dimension greater than two.

Recently, Luus and Lapidus (*20*, *22*) developed an averaging technique which overcomes the limitation of requiring the nonlinearities to be small, but this method is restricted to the analysis of a set of two first-order differential equations. Reid's extension of this averaging technique to a three-dimensional system by means of planar projections of the trajectories has been successful only in very special cases (*30*). Certain sets of highly nonlinear differential equations in canonical form can be analyzed by the nonlinear transformation technique of Dasarathy and Srinivasan (*9*) or the principle of harmonic balance term minimization developed by Ludeke and Wagner (*21*). Unfortunately, these two methods of analysis are not applicable to a set of first-order nonlinear differential equations which are not in canonical form.

Several approaches have been developed to determine the effect of parameter changes on system behavior by examining parameter sensitivity fuctions of either the solutions to differential and differential-difference equations (*7*, *16*, *19*, *33*, *36*, *39*, *41*) or the performance of controlled processes (*2*, *3*, *6*, *12*, *13*, *18*, *24*, *29*, *31*, *32*, *34*, *37*). In many applitions these techniques require extensive numerical calculations. Thus a more convenient approach is desired.

In this paper a parameter sensitivity analysis is developed by constructing an approximate analytical solution to the set of differential equations in terms of an oscillation whose envelope and phase are away from those of an approximate periodic solution. The effect of parameter changes on the approximate solution estimates the parameter sensitivity of the system.

STATEMENT OF THE PROBLEM

Consider a system described by the vector differential equation

$$\frac{d\mathbf{x}}{dt} = \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t, k) \tag{1}$$

The system is assumed to have a periodic solution with period $\tau = 2\pi/\omega$. It is required to determine the effect of a change in k on the general solution to Equation (1) from an arbitrary starting condition.

APPROXIMATE PERIODIC SOLUTION

Let us approximate the periodic solution to Equation (1) by the n-dimensional vector $\mathbf{y}$ whose elements are defined by

$$y_i = \sum_{j=0}^{m} a_{ij} \cos j(\varphi_e + \omega t) + \sum_{j=1}^{m} b_{ij} \sin j(\varphi_e + \omega t); \quad i = 1, 2, \cdots, n \tag{2}$$

where φ_e is the constant equilibrium phase, and the coefficients a_{ij} and b_{ij} are to be determined so that the average square error deviation from the true periodic solution is minimized. To obtain these coefficients we first define the vector

$$\boldsymbol{\lambda}' = (\lambda_1, \cdots, \lambda_{(2m+1)n}) = (a_{10}, \cdots, a_{n0}, a_{11}, \cdots, a_{nm}, b_{11}, \cdots, b_{nm}) \tag{3}$$

where $'$ is used to denote the transpose, and the averaged integrals

$$\left.\begin{aligned} Q_{ij}(\boldsymbol{\lambda}, \varphi_e, k) &= \frac{1}{T}\int_{t_0}^{t_0+T} [\dot{y}_i - f_i(\mathbf{y}, t, k)] \cos j(\varphi_e + \omega t)\, dt; \quad j = 0, 1, \cdots, m \\ P_{ij}(\boldsymbol{\lambda}, \varphi_e, k) &= \frac{1}{T}\int_{t_0}^{t_0+T} [\dot{y}_i - f_i(\mathbf{y}, t, k)] \sin j(\varphi_e + \omega t)\, dt; \quad j = 1, 2, \cdots, m \end{aligned}\right\} \tag{4}$$

where $i = 1, 2, \cdots, n$, t_0 is some arbitrary time, and T denotes the time over which the averaging is performed. For convenience we let the integrals defined by Equation (4) be the elements of a vector $\boldsymbol{\Phi}$ defined by

$$\boldsymbol{\Phi}'(\boldsymbol{\lambda}, \varphi_e, k) = (\Phi_1, \cdots, \Phi_{(2m+1)n}) = (Q_{10}, \cdots, Q_{n0}, Q_{11}, \cdots, Q_{nm}, P_{11}, \cdots, P_{nm}) \tag{5}$$

The best values for the coefficients a_{ij} and b_{ij} are obtained when the vector defined by Equation (5) vanishes over the period of $\mathbf{y}$, that is, $T = \tau$, to become the set of Galerkin equations (*5*, *8*, *11*, *14*, *15*, *40*).

$$\boldsymbol{\Phi}(\boldsymbol{\lambda}, \varphi_e, k) = \mathbf{0} \tag{6}$$

Equation (6) is also called the set of determining equations, since Cesari showed that if it is satisfied, the existence of a periodic solution is assured (*5*).

PARAMETER SENSITIVITY OF THE APPROXIMATE PERIODIC SOLUTION

In some cases Equation (6) can be solved analytically to yield $\boldsymbol{\lambda}$ as an explicit function of k. Then, differentiation of $\boldsymbol{\lambda}$ with respect to k gives the parameter sensitivity of the coefficients of the approximate periodic solution, and hence the sensitivity of the approximate periodic solution itself. If Equation (6) is difficult to solve analytically, a numerical method can be used. As an alternative to solving Equation (6) for several values of k, we may solve this equation only once for a specified value of the parameter, denoted by k_0, to yield

$$\boldsymbol{\lambda}_0 = \boldsymbol{\lambda}(k_0) \tag{7}$$

Then, to obtain both the coefficient vector $\boldsymbol{\lambda}$ and its parameter sensitivity $d\boldsymbol{\lambda}/dk$, we differentiate Equation (6) with respect to k; that is

$$\frac{d\boldsymbol{\Phi}}{dk} = \left(\frac{\partial \boldsymbol{\Phi}'}{\partial \boldsymbol{\lambda}}\right)' \frac{d\boldsymbol{\lambda}}{dk} + \frac{\partial \boldsymbol{\Phi}}{\partial k} = \mathbf{0} \tag{8}$$

Rearrangement of Equation (8) yields the differential equation

$$\frac{d\boldsymbol{\lambda}}{dk} = -\left[\left(\frac{\partial \boldsymbol{\Phi}'}{\partial \boldsymbol{\lambda}}\right)'\right]^{-1} \frac{\partial \boldsymbol{\Phi}}{\partial k} \tag{9}$$

if the inverse exists. Equation (9) gives both the parameter sensitivity of λ and, when integrated from the initial condition given by Equation (7), the solution of Equation (6) over a range of k.

If only the parameter sensitivity of the periodic solution is of interest we may stop here. However, since the primary concern is to determine the parameter sensitivity of the general solution corresponding to an arbitrary initial condition, it is necessary to continue the development.

APPROXIMATE GENERAL SOLUTION

Starting at an arbitrary initial condition, the general solution to Equation (1) is an oscillation whose period is usually time dependent and thus different from that of the periodic solution. The change in amplitude from period to period of such an oscillation is given by its envelope. Therefore we approximate the general solution, denoted by $\mathbf{z}(t)$, by a scalar envelope $v(t)$ and an n-dimensional vector $\mathbf{u}(t)$ whose elements u_i are functions of the same form as Equation (2) but with a time-dependent phase $\varphi(t)$; that is

$$z_i = v(t)\,u_i = v(t)\left\{\sum_{j=0}^{m} a_{ij}\cos j\,[\varphi(t)+\omega t] + \sum_{j=1}^{m} b_{ij}\sin j\,[\varphi(t)+\omega t]\right\} \quad (10)$$

The function $\varphi(t)$ is introduced to account for the difference between the periods of u_i and y_i. The time T in Equations (4) is taken to be the period of u_i.

If $\mathbf{z}$ approaches a stable periodic solution, we have from Equation (10) that

$$\lim_{t\to\infty} u_i = y_i \quad (11)$$

and that

$$\lim_{t\to\infty} v = 1 \quad (12)$$

The two unknowns, $v(t)$ and $\varphi(t)$, are now determined in a manner analogous to the variation of parameter technique for finding the general solution of a linear vector differential equation once the homogeneous solution is known (see reference *20*, p. 21). Substitution of the approximate solution as given by Equation (10) into Equation (1) yields

$$\dot{\mathbf{z}} = \dot{v}\,\mathbf{u} + v\,\dot{\mathbf{u}} = \mathbf{f}(v\,\mathbf{u},\ t,\ k) + \boldsymbol{\varepsilon} \quad (13)$$

where $\boldsymbol{\varepsilon}$ is an error term arising from the approximation. Multiplying Equation (13) by $\mathbf{u}'$ and rearranging terms yield the scalar differential equation for the envelope

$$\dot{v}\,\mathbf{u}'\mathbf{u} = -\mathbf{u}'[v\,\dot{\mathbf{u}} - \mathbf{f}(v\,\mathbf{u},\ t,\ k)] + \mathbf{u}'\boldsymbol{\varepsilon} \quad (14)$$

To develop a differential equation for φ we first express the time derivative of $\mathbf{z}$ by

$$\dot{\mathbf{z}} = \left(\frac{d\,v\,\mathbf{u}}{d(\varphi+\omega t)}\right)\left(\frac{d(\varphi+\omega t)}{dt}\right) = \frac{d\,v\,\mathbf{u}}{d(\varphi+\omega t)}(\dot{\varphi}+\omega) \quad (15)$$

Then, combining Equations (13) and (15), multiplying by $\dfrac{d\,v\,\mathbf{u}'}{d(\varphi+\omega t)}$, and rearranging terms, we get

$$\dot{\varphi}\left(\frac{d\,v\,\mathbf{u}'}{d(\varphi+\omega t)}\right)\left(\frac{d\,v\,\mathbf{u}}{d(\varphi+\omega t)}\right) = \left(\frac{d\,v\,\mathbf{u}'}{d(\varphi+\omega t)}\right) \times\left[-\omega\frac{d\,v\,\mathbf{u}}{d(\varphi+\omega t)} + \mathbf{f}(v\,\mathbf{u},\ t,\ k)\right] + \frac{d\,v\,\mathbf{u}'}{d(\varphi+\omega t)}\boldsymbol{\varepsilon} \quad (16)$$

If we let the average values of the weighted error terms in Equations (14) and (16) vanish over the assumed period of the oscillation T, the functions v and φ can be determined from the resulting equations:

$$\frac{1}{T}\int_{t_0}^{t_0+T}\dot{v}\,\mathbf{u}'\mathbf{u}\,dt = -\frac{1}{T}\int_{t_0}^{t_0+T}\mathbf{u}'[v\,\dot{\mathbf{u}} - \mathbf{f}(v\,\mathbf{u},\ t,\ k)]\,dt \quad (17)$$

and

$$\frac{1}{T}\int_{t_0}^{t_0+T}\dot{\varphi}\left(\frac{d\,v\,\mathbf{u}'}{d(\varphi+\omega t)}\right)\left(\frac{d\,v\,\mathbf{u}}{d(\varphi+\omega t)}\right)dt = \frac{1}{T}\int_{t_0}^{t_0+T}\left(\frac{d\,v\,\mathbf{u}'}{d(\varphi+\omega t)}\right)\left[-\omega\frac{d\,v\,\mathbf{u}}{d(\varphi+\omega t)} + \mathbf{f}(v\,\mathbf{u},\ t,\ k)\right]dt \quad (18)$$

Since Equations (17) and (18) are generally difficult to solve, estimates for v and φ are obtained instead, by introducing suitable approximations into these equations. First, at time t^*, where $t_0 \le t^* \le t_0 + T$, let v and φ take on some average values v^* and φ^*, representative of the envelope and phase which we assume do not change much over one period, and let $v = v^*$, $\varphi = \varphi^*$ over the entire period. At the same time, the tendency of v and φ to change over successive periods is given by the approximate derivatives $\dot{v}^*$ and $\dot{\varphi}^*$, which, from Equations (17) and (18), become

$$\dot{v}^* = \frac{-\dfrac{1}{T}\displaystyle\int_{t_0}^{t_0+T}\mathbf{u}'[v^*\,\dot{\mathbf{u}} - \mathbf{f}(v^*\,\mathbf{u},\ t,\ k)]\,dt}{\dfrac{1}{T}\displaystyle\int_{t_0}^{t_0+T}\mathbf{u}'\mathbf{u}\,dt} \quad (19)$$

and

$$\varphi^* = \frac{\dfrac{1}{T}\displaystyle\int_{t_0}^{t_0+T}\left(\frac{d\,v^*\,\mathbf{u}'}{d(\varphi^*+\omega t)}\right)\left[-\omega\frac{d\,v^*\,\mathbf{u}}{d(\varphi^*+\omega t)} + \mathbf{f}(v^*\,\mathbf{u},\ t,\ k)\right]dt}{\dfrac{1}{T}\displaystyle\int_{t_0}^{t_0+T}\left(\frac{d\,v^*\,\mathbf{u}'}{d(\varphi^*+\omega t)}\right)\left(\frac{d\,v^*\,\mathbf{u}}{d(\varphi^*+\omega t)}\right)dt} \quad (20)$$

If v and φ change over successive periods, the right-hand sides of Equations (19) and (20) yield nonzero values which indicate the change.

Since v^* and φ^* are taken to be constant on the right-hand sides of Equations (19) and (20), integration with respect to time in these equations can be performed explicitly. To carry out the integration we introduce three new vectors:

$$\hat{\lambda}' = \left(a_{10},\ \cdots,\ a_{no},\ \frac{a_{11}}{\sqrt{2}},\ \cdots,\ \frac{a_{nm}}{\sqrt{2}},\ \frac{b_{11}}{\sqrt{2}},\ \cdots,\ \frac{b_{nm}}{\sqrt{2}}\right) \quad (21)$$

$$\lambda_m' = (a_{11},\ 2a_{12},\ \cdots,\ ma_{nm},\ b_{11},\ 2b_{12},\ \cdots,\ mb_{nm}) \quad (22)$$

and

$$\Gamma' = (\Gamma^s_{11},\ \cdots,\ \Gamma^s_{1m},\ \cdots,\ \Gamma^s_{ij},\ \cdots,\ \Gamma^s_{n1},\ \cdots,\ \Gamma^s_{nm},\ \Gamma^c_{11},\ \cdots,\ \Gamma^c_{1m},\ \cdots,\ \Gamma^c_{ij},\ \cdots,\ \Gamma^c_{n1},\ \cdots,\ \Gamma^c_{nm}) \quad (23)$$

where

$$\Gamma^s_{ij} = \Gamma^s_{ij}(v^*\lambda, \varphi^*, k) = -\frac{1}{T}\int_{t_0}^{t_0+T} f_i(v^*\mathbf{u}, t, k)\sin j(\varphi^* + \omega t)\,dt \quad (24)$$

and

$$\Gamma^c_{ij} = \Gamma^c_{ij}(v^*\lambda, \varphi^*, k) = \frac{1}{T}\int_{t_0}^{t_0+T} f_i(v^*\mathbf{u}, t, k)\cos j(\varphi^* + \omega t)\,dt \quad (25)$$

Using Equations (5) and (21) to (25), Equations (19) and (20) give

$$\dot{v}^*\hat{\lambda}'\hat{\lambda} = -\lambda'\Phi(v^*\lambda, \varphi^*, k) \quad (26)$$

and

$$\dot{\varphi}^*\lambda_m'\lambda_m = \lambda_m'\left[-\omega\lambda_m + \frac{2}{v^*}\Gamma(v^*\lambda, \varphi^*, k)\right] \quad (27)$$

Equations (26) and (27) are used to approximate the functions v and φ over successive estimated periods. If, as was previously assumed, the functions v and φ do not change much over one period, they may be approximated by the time-dependent solutions to the differential equation counterparts of Equations (26) and (27); that is

$$\dot{v}\hat{\lambda}'\hat{\lambda} = -\lambda'\Phi(v\lambda, \varphi, k) \quad (28)$$

and

$$\dot{\varphi}\lambda_m'\lambda_m = \lambda_m'\left[-\omega\lambda_m + \frac{2}{v}\Gamma(v\lambda, \varphi, k)\right] \quad (29)$$

Equations (28) and (29) with Equation (10) provide an approximate solution to Equation (1) for an arbitrary initial condition. This approximate solution is a function of the parameter k and thereby incorporates any change in the parameter.

STABILITY OF THE PERIODIC SOLUTION

Equations (28) and (29) also specify the system's stability. For a nonautonomous system, the periodic solution is stable if Equations (28) and (29) show that $v \longrightarrow 1$ and $\varphi \longrightarrow \varphi_e$ as $t \longrightarrow \infty$. For an autonomous system, $\mathbf{f}$ is not explicitly periodic in t and therefore Equation (28) is independent of φ. In this case the phase φ is arbitrarily chosen to be zero, and Equation (28) is used alone to establish stability simply by following v as $t \longrightarrow \infty$.

If it is not possible to integrate Equations (28) and (29) analytically, the stability information can be readily obtained by the perturbation approach. To illustrate this procedure for an autonomous system, we introduce into Equation (28) the perturbation around $v = 1$:

$$v = 1 + \delta v \quad (30)$$

Then, expansion of Equation (28) in a Taylor series, and retaining terms up to second order, give

$$\delta\dot{v}\hat{\lambda}'\hat{\lambda} = -\lambda'\left(\frac{\partial\Phi'}{\partial v\lambda}\right)_{v=1}\lambda\delta v - \frac{1}{2}\lambda'\mathbf{S}\lambda(\delta v)^2 \quad (31)$$

where

$$\mathbf{S} = \begin{bmatrix} \lambda'\left(\dfrac{\partial^2\Phi_1}{\partial(v\lambda_i)\,\partial(v\lambda_j)}\right) \\ \vdots \\ \lambda'\left(\dfrac{\partial^2\Phi_{(2m+1)n}}{\partial(v\lambda_i)\,\partial(v\lambda_j)}\right) \end{bmatrix}_{v=1} \quad \begin{matrix} i = 1, 2, \cdots, (2m+1)n \\ j = 1, 2, \cdots, (2m+1)n \end{matrix} \quad (32)$$

is a $(2m + 1)n$ by $(2m + 1)n$ second derivative matrix and both matrices in Equation (31) are evaluated at a solution to Equation (6). From Equation (31) a sufficient condition for the asymptotic stability of the periodic solution is that the quadratic form $\lambda'\left(\dfrac{\partial\Phi'}{\partial v\lambda}\right)_{v=1}\lambda$ be positive.

When

$$\lambda'\left(\frac{\partial\Phi'}{\partial v\lambda}\right)_{v=1}\lambda = 0, \quad \lambda \neq \mathbf{0},$$

the periodic solution is semistable, stable from the outside if $\lambda'\mathbf{S}\lambda > 0$, and stable from the inside if $\lambda'\mathbf{S}\lambda < 0$. Moreover, variation of the parameter in these quadratic forms gives the parameter variation of $\delta\dot{v}$, thereby estimating the parameter sensitivity of the rate of convergence of $\mathbf{z}$ to a periodic solution.

SIMPLIFICATIONS FOR COMPLEX SYSTEMS

If Equation (6) does not readily yield a solution, implementation of the forgoing method of analysis is difficult and must be simplified. The approach taken is to start with a two-dimensional system and to extend to a higher dimensional system. Thus we first consider the set of differential equations

$$\left.\begin{aligned} \dot{x}_1 &= f_1(x_1, x_2, t, k) \\ \dot{x}_2 &= f_2(x_1, x_2, t, k) \end{aligned}\right\} \quad (33)$$

where $\mathbf{x} = \mathbf{0}$ is an isolated singularity different from a saddle point. The set of equations chosen to approximate the periodic solution is

$$\left.\begin{aligned} y_1 &= r\cos(\varphi_e + \omega t) \\ y_2 &= r\sin(\varphi_e + \omega t) + \alpha r\cos(\varphi_e + \omega t) \end{aligned}\right\} \quad (34)$$

where r is a positive constant and α is introduced to match stability of the singularity predicted by the nonlinear analysis to that known from linear analysis of Equations (33). The details of this matching procedure are presented in Example 3.

From Equations (3) and (22) the coefficient vectors λ and λ_m for Equations (34) become

$$\lambda'(r, \alpha) = (0, 0, r, \alpha r, 0, r) \quad (35)$$

and

$$\lambda_m'(r, \alpha) = (r, \alpha r, 0, r) \quad (36)$$

In this simplified procedure the coefficient r is not obtained by solving Equation (6) but rather by satisfying the conditions $v = 1$, $\varphi = \varphi_e$ in the envelope and phase equations (28) and (29); that is

$$\dot{v}r^2(1 + 0.5\alpha^2) = -r[Q_{11}(v\lambda(r, \alpha), \varphi, k) + \alpha Q_{21}(v\lambda(r, \alpha), \varphi, k) + P_{21}(v\lambda(r, \alpha), \varphi, k)] \quad (37)$$

$$\dot{\varphi}r^2(2 + \alpha^2) = -\omega r^2(2 + \alpha^2) + \frac{2r}{v}[\Gamma^s_{11}(v\lambda(r, \alpha), \varphi, k) + \alpha\Gamma^s_{21}(v\lambda(r, \alpha), \varphi, k) + \Gamma^c_{21}(v\lambda(r, \alpha), \varphi, k)] \quad (38)$$

If Equations (33) are autonomous, the envelope v is established from Equation (37), which is now independent of φ, and we may write

$$\dot{v}r^2(1 + 0.5\alpha^2) = -rF(v\lambda(r, \alpha), 0, k) \quad (39)$$

The coefficient r is determined as a function of k and α by solving Equation (39) after letting $v = 1$; that is

$$F(\lambda(r, \alpha), 0, k) = 0 \quad (40)$$

To obtain stability information by the perturbation approach, Equation (30) is substituted into Equation (39) to

TABLE 1. SIMPLIFIED STABILITY CRITERION FOR AUTONOMOUS SECOND-ORDER SYSTEMS ($r > 0$)

$\left.\frac{\partial F}{\partial v r}\right\|_{v=1} < 0;$		Unstable limit cycle
$\left.\frac{\partial F}{\partial v r}\right\|_{v=1} = 0;$	$\left.\frac{\partial^2 F}{(\partial v r)^2}\right\|_{v=1} > 0$	Semistable limit cycle, stable from outside
	$\left.\frac{\partial^2 F}{(\partial v r)^2}\right\|_{v=1} < 0$	Semistable limit cycle, stable from inside
$\left.\frac{\partial F}{\partial v r}\right\|_{v=1} > 0;$		Stable limit cycle

give the approximate envelope equation corresponding to Equation (31):

$$\delta \dot{v}(1 + .5\,\alpha^2) = -\left.\frac{\partial F}{\partial v r}\right|_{v=1} \delta v - \frac{r}{2}\left.\frac{\partial^2 F}{(\partial v r)^2}\right|_{v=1} (\delta v)^2 \quad (41)$$

The conditions of stability for Equations (34), predicted by Equation (41) using r obtained from Equation (40), are listed in Table 1. The partial derivatives in Table 1 yield the range of k, in terms of α, for the stability of a periodic solution. The coefficient α is then selected by matching the exact range of k for stability of the singularity of Equations (33), known from linear analysis, to the range of k specifying the instability of a periodic solution.

Since α is now known, r is a function of k only. A scalar sensitivity differential equation for r can be obtained by differentiating Equation (40) with respect to k and rearranging terms to give

$$\frac{dr}{dk} = -\frac{\partial F(\lambda(r, \alpha), 0, k)}{\partial k} \Big/ \frac{\partial F(\lambda(r, \alpha), 0, k)}{\partial r} \quad (42)$$

The initial condition of Equation (42), $r(k_0)$, results from the solution of Equation (40) at some value of k_0.

The parameter sensitivity of $\delta \dot{v}$ is indicated by the explicit parameter dependence of the partial derivatives in Table 1.

To extend such simplification to an n-dimensional system for which $\mathbf{f}(\mathbf{0}, t, k) = \mathbf{0}$, we use Equations (34) to approximate the periodic behavior of the first two state variables and approximate the periodic behavior of the remaining n-2 state variables by taking $m = 1$ in Equation (2):

$$y_i = a_{i0} + a_{i1} \cos(\varphi_e + \omega t) + b_{i1} \sin(\varphi_e + \omega t); \quad i = 3, 4, \cdots, n \quad (43)$$

The coefficients a_{i0}, a_{i1}, and b_{i1}, which are generally functions of k, α, r, and φ_e, are obtained from $3(n-2)$ determining equations. Replacing r and φ_e by vr and φ, respectively, Equation (43) then yields known functions in the first two differential equations; that is

$$\dot{x}_1 = f_1(x_1, x_2, y_3, y_4, \cdots, y_n, t, k)$$
$$\dot{x}_2 = f_2(x_1, x_2, y_3, y_4, \cdots, y_n, t, k)$$

A special class of systems which is not as difficult to analyze as the general system we have been considering, and requires less stringent approximations, is represented by the set of differential equations in canonical form:

$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= x_3 \\ &\cdots \\ \dot{x}_{n-1} &= x_n \\ \dot{x}_n &= f(\mathbf{x}, t, k) \end{aligned} \quad (44)$$

The approximate periodic solution to Equations (44) can be obtained from y_1 and its time derivatives, so we have more freedom to choose a better approximation than that suggested by Equations (34). For example, as a first approximation we may let

$$y_1 = a_{10} + a_{11} \cos(\varphi_e + \omega t) + b_{11} \sin(\varphi_e + \omega t) \quad (45)$$

and corresponding to this approximation the best choice for y_2 in the determining equations is the time derivative of y_1; that is

$$y_2 = -\omega a_{11} \sin(\varphi_e + \omega t) + \omega b_{11} \cos(\varphi_e + \omega t) \quad (46)$$

Similarly, $y_3, y_4, \cdots, y_n$ can be derived in a straightforward manner by successive differentiations.

EXAMPLES

The numerous approximations that have been introduced necessitate a careful test of the feasibility of this method of analysis in estimating the parameter sensitivity of the solutions of nonlinear differential equations with sufficient accuracy to be of practical value. For simplicity in illustrating the method of analysis, the first two examples are second-order systems written in the canonical form. The third example is a set of three first-order nonlinear differential equations describing a polymerization reaction in a continuous stirred-tank reactor.

Example I

To illustrate the sensitivity analysis and to test its applicability in analyzing two-dimensional autonomous nonlinear systems, let us consider the system

$$\left.\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= -x_1 - x_2\left(1 - \frac{x_2^2}{3} + k x_2^4\right) \end{aligned}\right\} \quad (47)$$

where k is a positive adjustable parameter.

To provide a means of selecting the frequency ω of the nonlinear periodic solution, the damping term in Equations (47) is dropped to give the equations for the harmonic oscillator:

$$\left.\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= -x_1 \end{aligned}\right\} \quad (48)$$

A reasonable choice for ω is the frequency of the periodic solution of Equations (48), which yields $\omega = -1$. Then, setting $\varphi = \varphi_e = 0$ because Equations (47) are autonomous, the first approximation ($m = 1$) to the nonlinear periodic solution chosen according to Equations (45) and (46) is

$$\left.\begin{aligned} y_1 &= a_{10} + a_{11} \cos(-t) + b_{11} \sin(-t) \\ y_2 &= a_{11} \sin(-t) - b_{11} \cos(-t) \end{aligned}\right\} \quad (49)$$

Since $y_2 = \dot{y}_1$, the determining equations corresponding to the first state variable are identically zero. The determining equations for the other state variable are evaluated from Equations (6) and (47). Taking $i = 2$, $j = 0$ we get

$$\Phi_2 = Q_{20}(\lambda, 0, k) = \frac{1}{\tau}\int_{t_0}^{t_0+\tau} \left[\dot{y}_2 + y_1 + y_2\left(1 - \frac{y_2^2}{3} + k y_2^4\right)\right] dt = 0 \quad (50)$$

Substitution of Equations (49) into Equation (50) and integration yield

$$Q_{20}(\lambda, 0, k) = a_{10} = 0 \quad (51)$$

Taking $i = 2$, $j = 1$, Equations (6) and (47) give

$$\Phi_4 = Q_{21}(\lambda, 0, k) = \frac{1}{\tau}\int_{t_0}^{t_0+\tau} \left[\dot{y}_2 + y_1 + y_2\left(1 - \frac{y_2^2}{3} + k y_2^4\right)\right] \cos(-t)\, dt = 0 \quad (52)$$

and

$$\Phi_6 = P_{21}(\lambda, 0, k)$$

$$= \frac{1}{\tau}\int_{t_0}^{t_0+\tau}\left[\dot{y}_2 + y_1 + y_2\left(1 - \frac{y_2^2}{3} + ky_2^4\right)\right]\sin(-t)\,dt = 0 \quad (53)$$

Substitution of Equations (49) into Equations (52) and (53), integration, and rearrangement of terms give

$$Q_{21}(\lambda, 0, k) = -\frac{b_{11}}{8}\left[\frac{5}{2}k(a_{11}^2 + b_{11}^2)^2 - (a_{11}^2 + b_{11}^2) + 4\right] = 0 \quad (54)$$

$$P_{21}(\lambda, 0, k) = \frac{a_{11}}{8}\left[\frac{5}{2}k(a_{11}^2 + b_{11}^2)^2 - (a_{11}^2 + b_{11}^2) + 4\right] = 0 \quad (55)$$

A solution to Equations (54) and (55) is related by one equation in two unknowns:

$$a_{11}^2 + b_{11}^2 = \frac{1 \pm\sqrt{1 - 40k}}{5k};\ 0 < k \leq 0.025 \quad (56)$$

This gives freedom to choose one of the unknowns. For simplicity we let $b_{11} = 0$. Then, from Equations (54) and (55) the only determining equation which is not identically zero is

$$P_{21}(\lambda, 0, k) = \frac{5}{16}ka_{11}^5 - \frac{a_{11}^3}{8} + \frac{a_{11}}{2} = 0 \quad (57)$$

and from Equation (56)

$$a_{11} = \sqrt{\frac{1 \pm\sqrt{1 - 40k}}{5k}};\ 0 < k \leq 0.025 \quad (58)$$

From Equations (49), a_{11} is identified as the radius of the approximate limit cycle

$$\left.\begin{aligned} y_1 &= a_{11}\cos(-t) \\ y_2 &= a_{11}\sin(-t) \end{aligned}\right\} \quad (59)$$

The parameter sensitivity of the limit cycle can be obtained by differentiating Equation (58) with respect to k or, more simply, by differentiating Equation (57); that is

$$\frac{da_{11}}{dk} = \frac{-5a_{11}^5}{25ka_{11}^4 - 6a_{11}^2 + 8} \quad (60)$$

where a_{11} is given by Equation (58). When a_{11} and da_{11}/dk in Equations (58) and (60), respectively, are plotted with k as independent variable, Figures 1 and 2 result. From Figure 1 we see that for $k = 0.025$ a single limit cycle of radius $a_{11} = 2\sqrt{2}$ is predicted, and as k is decreased, two limit cycles are predicted. When $k \longrightarrow 0$ the outer limit cycle radius becomes infinitely large and the inner limit cycle radius approaches 2. For $k > 0.025$ there are no real values of a_{11} and we conclude that a limit cycle cannot exist. Figure 2 shows the parameter sensitivity of the limit cycle radii as a function of k. The outer limit cycle radius is seen to be more sensitive to a parameter change than the inner limit cycle radius, both cycles becoming very sensitive as $k \longrightarrow 0.025$.

We now estimate the behavior of the general solution to Equations (47) by means of the envelope perturbation Equation (31). Since Equations (47) are autonomous, the phase equation is not required. The vector of the coefficients of Equations (59) is

$$\lambda' = (0, 0, a_{11}, 0, 0, a_{11}) \quad (61)$$

and the vector $\Phi(v\lambda, 0, k)$ becomes

$$\Phi'(v\lambda, 0, k) = (0, 0, 0, 0, 0, P_{21}(v\lambda, 0, k)) \quad (62)$$

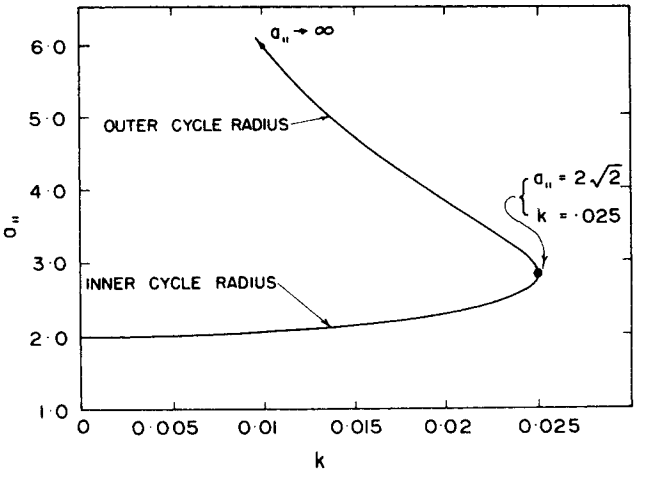

Fig. 1. Approximate radii of limit cycles of Equations (47).

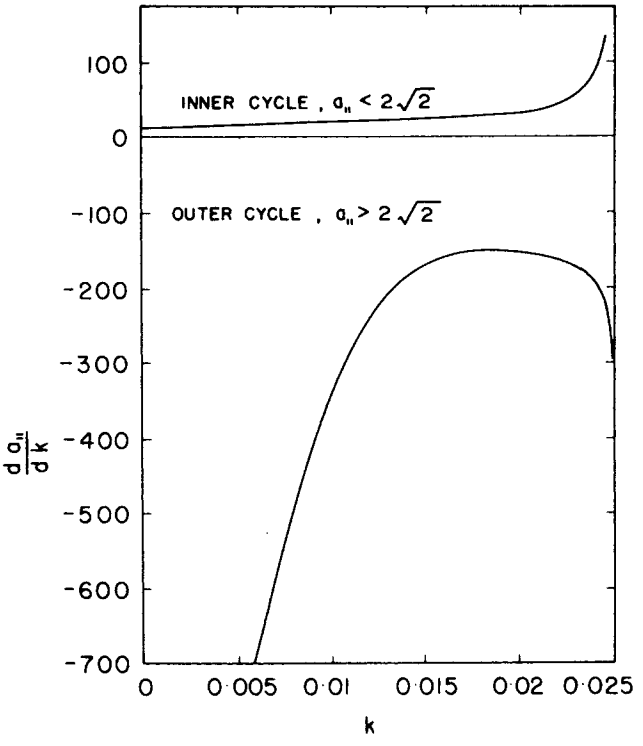

Fig. 2. Parameter sensitivities of radii of limit cycles of Equations (47).

where, from Equation (57)

$$P_{21}(v\lambda, 0, k) = \frac{5}{16}kv^5a_{11}^5 - v^3\frac{a_{11}^3}{8} + v\frac{a_{11}}{2} \quad (63)$$

The first derivative quadratic form of Equation (31) is then evaluated to be

$$\lambda'\left(\frac{\partial\Phi'}{\partial v\lambda}\right)_{v=1}\lambda = a_{11}^2\left.\frac{\partial P_{21}(v\lambda, 0, k)}{\partial va_{11}}\right|_{v=1} = a_{11}^2\left[\frac{25}{16}ka_{11}^4 - \frac{3}{8}a_{11}^2 + \frac{1}{2}\right] \quad (64)$$

Similarly, the second derivative quadratic form of Equation (31) is

$$\lambda' S\lambda = a_{11}^3\left.\frac{\partial^2 P_{21}(v\lambda, 0, k)}{(\partial va_{11})^2}\right|_{v=1} = a_{11}^3\left[\frac{25}{4}ka_{11}^3 - \frac{3}{4}a_{11}\right] \quad (65)$$

Equation (31) is then simplified using Equations (64) and (65) and dividing by a_{11}^2 to obtain

$$\delta\dot{v} = -\left[\frac{25}{16}ka_{11}^2 - \frac{3}{8}a_{11}^2 + \frac{1}{2}\right]\delta v - \frac{a_{11}}{2}\left[\frac{25}{4}ka_{11}^3 - \frac{3}{4}a_{11}\right](\delta v)^2 \quad (66)$$

Equation (66) is of the same form as Equation (41) and stability can be determined from Table 1. For $k = 0.025$, $a_{11} = 2\sqrt{2}$, the coefficient of δv in Equation (66) vanishes but the coefficient of $(\delta v)^2$ is negative. Therefore the limit cycle with radius $a_{11} = 2\sqrt{2}$ is semistable, stable from the outside. This result is confirmed by numerical integration of Equations (47) for which the computed and predicted orbits are given in Figure 3. For $0 < k < 0.025$, Equation (66) establishes that the coefficient of δv is positive when $2 < a_{11} < 2\sqrt{2}$ and is negative when $a_{11} > 2\sqrt{2}$. Therefore the inner limit cycle is unstable while the outer limit cycle is stable. Figure 4 shows good agreement between the computed and predicted limit cycles for $k = 0.02$. If $k > 0.025$, no limit cycle exists and the stable equilibrium point $x_1 = x_2 = 0$ is approached from every point in the $x_1 - x_2$ plane.

In addition to its use for establishing stability information, the partial derivative in Equation (64) is used to estimate the rate at which the general solution either leaves or approaches a limit cycle as k is varied. Figure 5 shows that the stable outer limit cycle is approached rapidly for small k but that this rate of approach decreases as $k \longrightarrow 0.025$. Alternatively, the solution leaves the unstable inner limit cycle with a rate which is relatively slower and which varies slightly over the range $0 < k < 0.025$. The confirmation of these predicted results by numerical integration of Equations (47) gives us confidence in using this method to analyze other two-dimensional autonomous systems.

Example 2

To test this method of analysis for nonautonomous systems, let us determine the limit cycle behavior of the

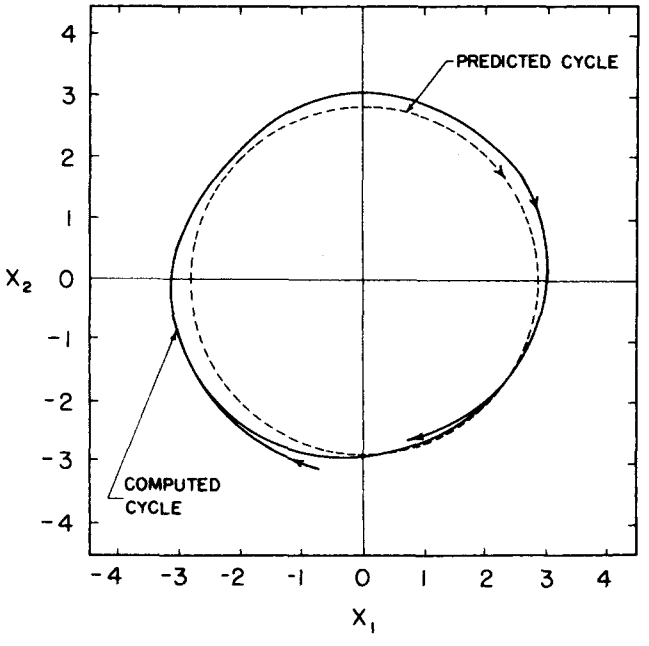

Fig. 3. Predicted and computed limit cycles of Equations (47); $k = 0.025$.

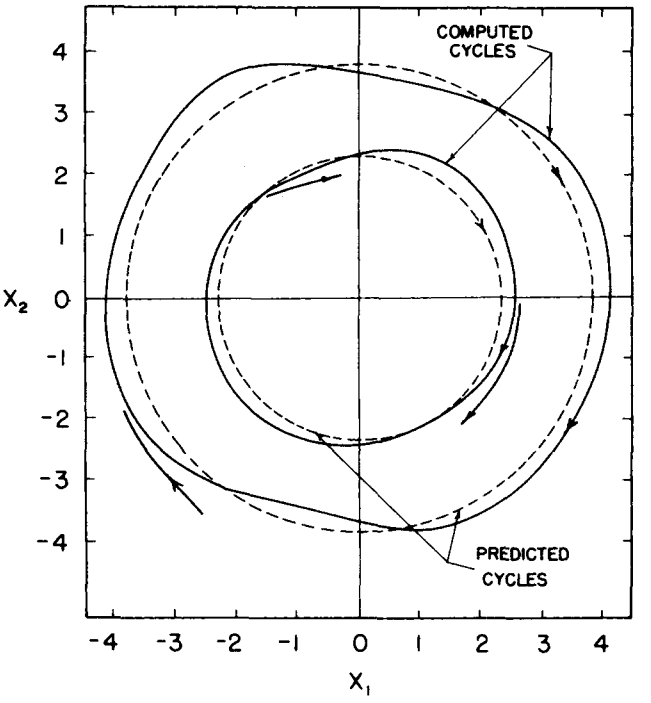

Fig. 4. Predicted and computed limit cycles of Equations (47); $k = 0.02$.

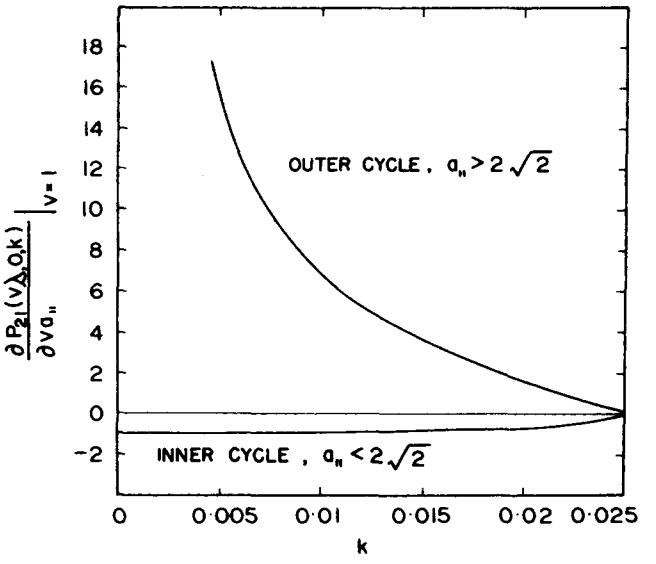

Fig. 5. Parameter variation of general solution's rate of approaching or leaving limit cycles of Equations (47).

van der Pol equation with a forcing function whose frequency is equal to the frequency of the unforced system. Such a system is written in the canonical form

$$\left.\begin{aligned}\dot{x}_1 &= x_2 \\ \dot{x}_2 &= -x_1 + \varepsilon(1 - x_1^2)x_2 + A\sin\omega t\end{aligned}\right\} \quad (67)$$

where $\varepsilon > 0$, $\omega = -1$ and A is the amplitude of the forcing function. It has been shown that for $A > 0$ and $\varepsilon > 0$, a solution of Equations (67) is a stable limit cycle whose amplitude is bounded and can be accurately predicted by the averaging technique (*20*). In this example we show further that for certain values of A and ε, an unstable limit cycle is contained in this stable limit cycle.

From Equations (45) and (46) a first approximation to the periodic solution of Equations (67) is chosen to be

$$\left.\begin{aligned} y_1 &= a_{10} + a_{11}\cos(\varphi_e - t) + b_{11}\sin(\varphi_e - t) \\ y_2 &= a_{11}\sin(\varphi_e - t) - b_{11}\cos(\varphi_e - t) \end{aligned}\right\} \quad (68)$$

Since $\dot{y}_1 = y_2$, the determining equations for the first state variable are identically zero. The determining equations for the remaining state variable are evaluated from Equations (6) and (67), which, for $i = 2$, $j = 0$, gives

$$\Phi_2 = Q_{20}(\lambda, \varphi_e, k) = \frac{1}{\tau}\int_{t_0}^{t_0+\tau} [\dot{y}_2 + y_1 - \varepsilon(1 - y_1^2)y_2 + A\sin t]\,dt = 0 \quad (69)$$

Substitution of Equations (68) into Equation (69) and integration yield

$$Q_{20}(\lambda, \varphi_e, k) = a_{10} = 0 \quad (70)$$

With $i = 2$, $j = 1$ the determining equations are

$$\Phi_4 = Q_{21}(\lambda, \varphi_e, k) = \frac{1}{\tau}\int_{t_0}^{t_0+\tau} [\dot{y}_2 + y_1 - \varepsilon(1 - y_1^2)y_2 + A\sin t]\cos(\varphi_e - t)\,dt = 0 \quad (71)$$

and

$$\Phi_6 = P_{21}(\lambda, \varphi_e, k) = \frac{1}{\tau}\int_{t_0}^{t_0+\tau} [\dot{y}_2 + y_1 - \varepsilon(1 - y_1^2)y_2 + A\sin t]\sin(\varphi_e - t)\,dt = 0 \quad (72)$$

Substitution of Equations (68) and (70) into Equations (71) and (72) and integration yield

$$Q_{21}(\lambda, \varphi_e, k) = \frac{\varepsilon}{2}b_{11} - \frac{\varepsilon}{8}a_{11}^2 b_{11} - \frac{\varepsilon}{8}b_{11}^3 + \frac{A}{2}\sin\varphi_e = 0 \quad (73)$$

and

$$P_{21}(\lambda, \varphi_e, k) = -\frac{\varepsilon}{2}a_{11} + \frac{\varepsilon}{8}a_{11}b_{11}^2 + \frac{\varepsilon}{8}a_{11}^3 - \frac{A}{2}\cos\varphi_e = 0 \quad (74)$$

Equations (73) and (74) relate the three unknowns a_{11}, b_{11}, and φ_e and give freedom to choose a feasible solution as was the case of the previous example. If we let $b_{11} = 0$, Equations (73) and (74) become

$$\frac{A}{2}\sin\varphi_e = 0 \quad (75)$$

and

$$\frac{\varepsilon}{8}a_{11}^3 - \frac{\varepsilon}{2}a_{11} - \frac{A}{2}\cos\varphi_e = 0 \quad (76)$$

Since $A \neq 0$, Equation (75) yields $\sin\varphi_e = 0$; that is, $\varphi_e = 0$ or $\varphi_e = \pi$. By choosing an adjustable parameter to be

$$k = \frac{A}{\varepsilon}\cos\varphi_e \quad (77)$$

one can write Equation (76) as

$$a_{11}^3 - 4a_{11} - 4k = 0 \quad (78)$$

where, from Equations (68), a_{11} is the radius of the approximate limit cycle:

$$\left.\begin{aligned} y_1 &= a_{11}\cos(\varphi_e - t) \\ y_2 &= a_{11}\sin(\varphi_e - t) \end{aligned}\right\} \quad (79)$$

Equation (78) can be solved analytically but such a procedure is cumbersome. Instead, we differentiate Equation (78) with respect to k and obtain the sensitivity differential equation, which through numerical integration directly yields a_{11} and da_{11}/dk. Performing the differentiation and rearranging terms, we get

$$\frac{da_{11}}{dk} = \frac{4}{3a_{11}^2 - 4}; \quad a_{11} \neq \sqrt{\frac{4}{3}} \quad (80)$$

Assuming $a_{11} \geq 0$ and setting $k = 0$ in Equation (78) yield two feasible initial conditions for Equation (80):

$$a_{11}(0) = 0 \quad (81)$$

and

$$a_{11}(0) = 2 \quad (82)$$

With initial condition (82), Equation (80) is integrated forward with $k \geq 0$ and backward in the range $\sqrt{\frac{4}{3}} < a_{11} < 2$ corresponding to $-0.77 < k < 0$. With initial condition (81), Equation (80) is integrated backward in the range $0 \leq a_{11} < \sqrt{\frac{4}{3}}$ for $-0.77 < k \leq 0$. Figures 6 and 7 show the limit cycle radii and the absolute values of their parameter sensitivities, respectively, predicted from this integration.

In order that a limit cycle be stable, it is necessary that its equilibrium phase be stable. This is established through the phase equation (29) with the coefficient vectors defined by Equations (3) and (22):

$$\lambda' = (0, 0, a_{11}, 0, 0, a_{11}) \quad (83)$$

and

$$\lambda_m' = (a_{11}, 0, 0, a_{11}) \quad (84)$$

Substitution of Equations (83) and (84) into Equation (29) yields

$$\dot{\varphi}a_{11}^2 = a_{11}^2 + \frac{a_{11}}{v}[\Gamma_{11}^s(v\lambda, \varphi, k) + \Gamma_{21}^c(v\lambda, \varphi, k)] \quad (85)$$

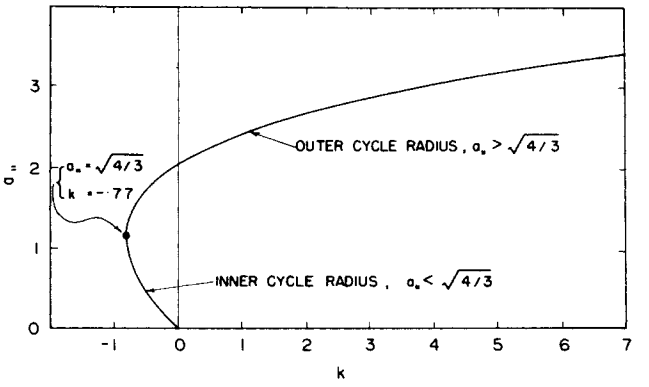

Fig. 6. Predicted radii of limit cycles of forced van der Pol Equations (67).

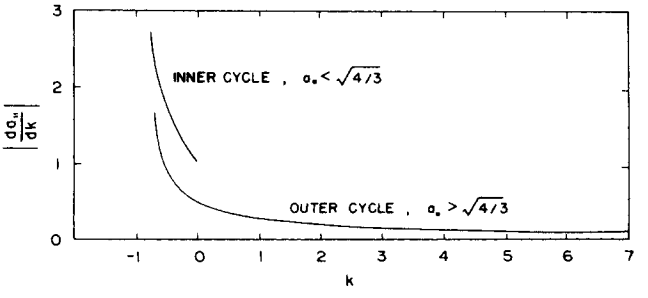

Fig. 7. Absolute values of parameter sensitivities of predicted radii of limit cycles of forced van der Pol Equations (67).

Since $u_i = y_i$ with time-dependent phase, the integrals Γ^s_{11} and Γ^c_{21}, defined by Equations (24) and (25), are evaluated using Equations (67) and (79) to be

$$\Gamma^s_{11} = -\frac{1}{T}\int_{t_0}^{t_0+T} v^* y_2 \sin(\varphi^* - t)\,dt = -v^*\frac{a_{11}}{2} \quad (86)$$

and

$$\Gamma^c_{21} = \frac{1}{T}\int_{t_0}^{t_0+T} [-v^* y_1 + \varepsilon(1 - v^{*2} y_1^2) v^* y_2 - A \sin t] \cos(\varphi^* - t)\,dt = -v^*\frac{a_{11}}{2} - \frac{A}{2}\sin\varphi^* \quad (87)$$

Allowing v^* and φ^* to be the time-dependent variables v and φ and combining Equations (85), (86), and (87), we get, after simplifying

$$\dot{\varphi} = \frac{-A}{2 v a_{11}} \sin\varphi \quad (88)$$

The condition for stability of the limit cycle is readily established if we introduce the perturbations

$$\left.\begin{aligned} v &= 1 + \delta v \\ \varphi &= \varphi_e + \delta\varphi \end{aligned}\right\} \quad (89)$$

into Equation (88); that is

$$\delta\dot{\varphi} = \frac{-A}{2(1+\delta v) a_{11}} (\sin\varphi_e \cos\delta\varphi + \cos\varphi_e \sin\delta\varphi) \quad (90)$$

If the limit cycle is stable, $\delta v \longrightarrow 0$ and $\delta\varphi \longrightarrow 0$, and since $\sin\varphi_e = 0$, Equation (90) is approximated by

$$\delta\dot{\varphi} = \frac{-A}{2a_{11}} \cos\varphi_e \delta\varphi \quad (91)$$

Equations (91) and (77) show that a limit cycle is stable provided $k > 0$ and unstable provided $k < 0$. The parameter k is positive for $\varphi_e = 0$ or $\varphi_e = \pi$ if A is positive or negative, respectively. Therefore the stable limit cycle is expected with $\varphi_e = 0$ and $A > 0$ or with $\varphi_e = \pi$ and $A < 0$. Integration of Equations (67) confirms the existence of this stable limit cycle. Although there are two positive values of a_{11} for $-0.77 < k < 0$, the two concentric unstable limit cycles predicted by this cannot exist. We therefore conclude that the determining equations have an extraneous solution. Backward integration of the system equations (67) confirms the existence of the smaller of the two predicted unstable limit cycles when A and ε are such that $-0.77 < k < 0$. This unstable limit cycle appears with $\varphi_e = \pi$ and $A > 0$ or with $\varphi_e = 0$ and $A < 0$.

The numerically computed limit cycles of the forced van der Pol equation are nearly circular orbits in the $x_1 - x_2$ plane. Therefore the computed limit cycle radius is taken to be the maximum value of x_1. When this maximum value is compared to the predicted radius a_{11}, agreement to within 3% is found when $\varepsilon = 1$ and $-7 \leq A \leq 7$. Of particular interest is the accurate prediction of the small unstable limit cycle whose existence goes unnoticed by forward integration of Equations (67).

Example 3

To test the application of the sensitivity analysis to a set of three first-order nonlinear differential equations, let us consider the monomer terminated addition polymerization in a continuous stirred-tank reactor which was studied by means of a Lyapunov function method by Warden, Aris, and Amundson (*42*). They investigated the asymptotic stability of a given steady state of the system for a choice of a proportional control constant and indicated a region of stability on projected planes in the three-dimensional state space. We give a more detailed analysis of this system and explicitly show the dependence of the region of stability on the control parameter.

The equations for heat and mass balance in dimensionless coordinates as derived by Warden et al. become

$$\dot{T} = -T - kT(T + 0.25) - 0.002[1 - (1+M)\xi^6] - 0.802[1 - (1+M)(1+V)\xi^{12}] \quad (92)$$

$$\dot{M} = -M + 0.04[1 - (1+M)\xi^6] + 4.02[1 - (1+M)(1+V)\xi^{12}] \quad (93)$$

$$\dot{V} = -V - 2[1 - (1+M)\xi^6] + [1 - (1+M)(1+V)\xi^{12}] \quad (94)$$

where T is the deviation from steady state dimensionless temperature, $\xi = \exp\frac{T}{1+T}$, k is the proportional control parameter, M is the deviation from steady state dimensionless monomer concentration, and V is the deviation from steady state dimensionless zeroth moment of the polymer concentration distribution. Therefore the steady state is given by $T = M = V = 0$.

To start the analysis let us introduce the approximations

$$\xi^6 = 1 + 6T + 12T^2 + 6T^3 \quad (95)$$

and

$$\xi^{12} = 1 + 12T + 60T^2 + 156T^3 \quad (96)$$

Using Equations (95) and (96) in the heat and mass balance equations (92), (93), and (94), and retaining terms up to third order, we get

$$\dot{T} = (8.632 - 0.250k)T + 0.804M + 0.802V + (48.14 - k)T^2 + 9.63TM + 9.62TV + 0.802MV + 125.01T^3 + 48.14T^2M + 9.62TMV + 48.12T^2V \quad (97)$$

$$\dot{M} = -48.48T - 5.06M - 4.02V - 241.68T^2 - 48.48TM - 48.24TV - 4.02MV - 627.36T^3 - 241.68T^2M - 241.20T^2V - 48.24TMV \quad (98)$$

$$\dot{V} = M - 2V - 36T^2 - 12TV - MV - 144T^3 - 36T^2M - 60T^2V - 12TMV \quad (99)$$

An attempt to estimate the periodic behavior of T, M, and V by y_1, y_2, and y_3 of Equation (2) yields determining equations which are difficult to solve, even numerically. Instead of using this approach we employ the method outlined by Equations (33) to (43) and introduce further approximations so that numerical computation is unnecessary.

Stability information is first obtained by linearizing Equations (97), (98), and (99) in the vicinity of the origin, $T = M = V = 0$. Application of the Routh-Hurwitz test to the linearized system establishes that the origin is asymptotically stable if $k > 15.92$. Since we wish to investigate the parameter variation effect on the size of the stability region, the system is examined near $k = 15.92$. The complex roots of the linear system characteristic equation and the clockwise rotation of trajectories in the T-M plane show that ω varies from -4.5 to -5.2 for $15 \leq k \leq 22$. For the investigation we choose $\omega = -5$ as a resonable approximation to the frequency of the oscillation. The characteristic equation also shows that the origin is not a saddle point if $k > 2.56$, so the approximate periodic solutions corresponding to Equations (34) and (43) can be used in the parameter range of interest. Since the continuous stirred-tank reactor is an autonomous system, we let $\varphi = \varphi_e = 0$, and Equations (34) and (43) become

$$y_1 = r\cos(-5t) \quad (100)$$

$$y_2 = r\sin(-5t) + \alpha r\cos(-5t) \quad (101)$$

$$y_3 = a_{30} + a_{31}\cos(-5t) + b_{31}\sin(-5t) \quad (102)$$

With $i = 3$, $m = 1$, Equations (6) and (99) to (102) yield the determining equations for the coefficients of Equation (102). It is assumed for simplicity in the calculations that α is negligibly small, a_{30} can be dropped, and that a_{31} and b_{31} are linear functions of r which vanish at $r = 0$ and whose slopes for all r are represented with sufficient accuracy by their slopes at $r = 0.1$. This gives

$$y_3 = 0.19r \cos(-5t) + 0.09r \sin(-5t) \quad (103)$$

To determine r and stability of the periodic solution, the envelope equation (37) is required. The functions Q_{11}, Q_{21}, and P_{21} in Equation (37) are obtained by first substituting Equations (97), (98), (100), (101), and (103) into Equations (4) and integrating to give

$$Q_{11}(\lambda(r, \alpha), 0, k) = (0.125k - 4.40)r - 50.44r^3 - \alpha(0.08r + 18.75r^3) \quad (104)$$

$$Q_{21}(\lambda(r, \alpha), 0, k) = 22.12r + 253.66r^3 + \alpha(2.53r + 94.04r^3) \quad (105)$$

$$P_{21}(\lambda(r, \alpha), 0, k) = 2.71r + 34.06r^3 + \alpha(2.50r + 0.54r^3) \quad (106)$$

Replacing r by vr in Equations (104) to (106) and combining these with Equation (37), we get the envelope equation

$$\dot{v}r^2(1 + 0.5\alpha^2) = -r[(0.125k - 1.69 + 24.54\alpha + 2.53\alpha^2)vr - (16.38 - 235.45\alpha - 94.04\alpha^2)v^3r^3] = -rF(v\lambda(r, \alpha), 0, k) \quad (107)$$

Substituting $v = 1$ into Equation (107), we solve for r as a function of k and α; that is

$$r = \sqrt{\frac{0.125k - 1.69 + 24.54\alpha + 2.53\alpha^2}{16.38 - 235.45\alpha - 94.04\alpha^2}} \quad (108)$$

To determine the stability of the approximate periodic solution we form the first partial derivative of F on the right-hand side of Equation (107) with respect to vr, evaluated at $v = 1$

$$\left.\frac{\partial F(v\lambda(r, \alpha), 0, k)}{\partial vr}\right|_{v=1} = 0.125k - 1.69 + 24.54\alpha + 2.53\alpha^2 - 3(16.38 - 235.45\alpha - 94.04\alpha^2)r^2 \quad (109)$$

Substitution of Equation (108) into Equation (109) yields

$$\left.\frac{\partial F(v\lambda(r, \alpha), 0, k)}{\partial vr}\right|_{v=1} = -2(0.125k - 1.69 + 24.54\alpha + 2.53\alpha^2) \quad (110)$$

Then, from Equation (110) and Table 1, we expect that an unstable periodic solution surrounds a stable origin if

$$k > \frac{1.69 - 24.54\alpha - 2.53\alpha^2}{0.125} \quad (111)$$

Since the origin is known from the linear analysis to be stable for $k > 15.92$, two possible values of α determined from inequality (111) are

$$\alpha = -0.012 \quad \text{and} \quad \alpha = -9.69 \quad (112)$$

The coefficient α is assumed small so $\alpha = -0.012$ is substituted into Equations (108) and (110) to give

$$r = \sqrt{\frac{0.125k - 1.99}{19.30}}; \quad k > 15.92 \quad (113)$$

$$\left.\frac{\partial F(v\lambda(r, -0.012), 0, k)}{\partial vr}\right|_{v=1} = 3.98 - 0.25k < 0; \quad k > 15.92 \quad (114)$$

Therefore an unstable periodic solution in the T-M plane is approximated by Equations (100), (101), and (113) if $k > 15.92$. Such an unstable periodic solution is a projection into the T-M plane of the boundary of the approximate region of stability in the three-dimensional T-M-V space. The approximation to the boundary of the stability region in the T-V plane is given by Equations (100), (103), and (113). From Equation (113) we expect this region of stability to increase for increasing k. Moreover, since the magnitude of the partial derivative in Equation (114) increases with k, the rate of convergence of a solution to the origin is expected to increase with k. Numerical integration of Equations (92), (93), and (94) confirms both that a region of stability of increasing size surrounds the origin, and that inside this region the rate of convergence of the solution to the origin increases as k increases beyond 15.92. If $k < 15.92$ the origin is unstable. In this case, since Equation (113) shows that r is imaginary, a limit cycle around the origin does not exist. For $k = 18$, Figure 8 shows the numerically computed region of stability and the region of stability predicted by $\alpha = -0.012$ and Equations (100), (101), (103), and (113). These results differ from those obtained by Warden et al., who state that the origin is a stable node for $k > -9.4$, is a saddle point for $k = -9.4$, and that the system is stable in the entire half space, $T > -1$, if $k = -9$ (*42*).

Stability information predicted without error correction is evaluated by substituting $\alpha = 0$ into Equations (108) and (110) to give

$$r = \sqrt{\frac{0.125k - 1.69}{16.38}}; \quad k > 13.52 \quad (115)$$

$$\left.\frac{\partial F(v\lambda(r, 0), 0, k)}{\partial vr}\right|_{v=1} = 3.38 - 0.25k < 0; \quad k > 13.52 \quad (116)$$

Comparison of Equations (115) and (116) to Equations (113) and (114), respectively, shows that without error correction the critical value of k for stability is underestimated by 15% and that for $k > 15.92$ the predicted region of stability is larger than that predicted using $\alpha = -0.012$. Figure 8 demonstrates the more conservative, and therefore safer, estimate of the stability region obtained with error correction.

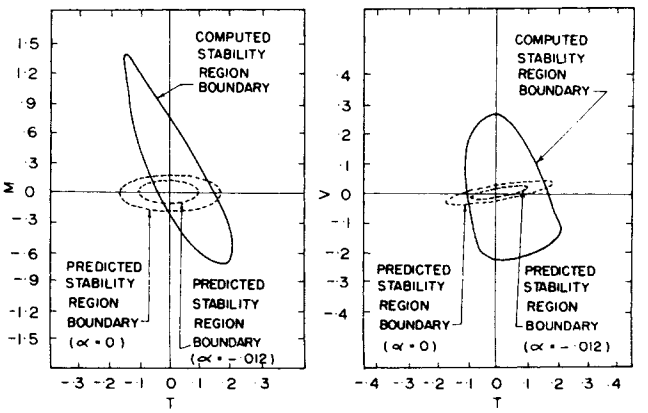

Fig. 8. Predicted and computed stability regions for Equations (92), (93), and (94); $k = 18$.

The choice of $\omega = -5$ for the frequency of the oscillation resulted in satisfactory estimates of the behavior of the continuous stirred-tank reactor in the parameter range $15 \leq k \leq 22$. For other k, system behavior is simply obtained by numerical integration with Equations (113) and (114) as a useful guide.

CONCLUSIONS

The parameter sensitivity of a system is adequately predicted by examining the parameter variation effect on the approximate solution to the set of differential equations describing the system. This method of analysis, although more difficult to apply than the averaging technique, gives identical results for two-dimensional systems. But, it has the advantage of being applicable to three-dimensional systems, as was illustrated by the analysis of the monomer terminated addition polymerization in a continuous stirred-tank reactor. Once the difficulty of solving the set of determining equations is overcome, the method should be also effective for nonlinear systems of dimensionality greater than three.

ACKNOWLEDGMENT

Financial assistance from the National Research Council of Canada was gratefully received by R. J. Rayzak. This work made use of the computer facilities at the University of Toronto.

NOTATION

a = coefficient in Equations (2)
A = amplitude of sinusoidal forcing function of van der Pol equation
b = coefficient in Equations (2)
c = superscript denoting integral as defined in Equation (25)
d = differential notation
e = subscript denoting equilibrium
f = arbitrary function
$\mathbf{f}$ = n-dimensional vector of arbitrary functions
F = scalar function of elements of Φ
i = subscript denoting the state variable or column of matrix
j = coefficient or subscript in Equations (2); subscript denoting row of matrix
k = adjustable parameter
m = coefficient or subscript denoting term in series approximation
n = system dimensionality
P = function as defined by Equations (4)
Q = function as defined by Equations (4)
r = coefficient in approximate periodic solution as defined by Equations (34)
s = superscript denoting integral as defined in Equation (24)
$\mathbf{S}$ = $(2m + 1)n$ by $(2m + 1)n$ second derivative matrix
t = time
t_0 = arbitrary time
t^* = time in interval $[t_0, t_0 + T]$
T = period of $\mathbf{u}$; deviation from steady state dimensionless temperature
$\mathbf{u}$ = n-dimensional vector of oscillating part of $\mathbf{z}$
v = envelope of approximate general solution
v^* = envelope evaluated at t^*
V = deviation from steady state dimensionless zeroth moment of polymer concentration distribution
$\mathbf{x}$ = n-dimensional space coordinate vector
$\mathbf{y}$ = n-dimensional approximate periodic solution vector as defined by Equations (2)
$\mathbf{z}$ = n-dimensional approximate general solution vector as defined by equation (10)

Greek Letters

α = correction coefficient in Equations (34)
$\mathbf{\Gamma}$ = $2mn$-dimensional vector as defined by Equation (23)
ε = parameter in forced van der Pol equation
$\boldsymbol{\varepsilon}$ = n-dimensional error term in Equation (13)
λ = $(2m + 1)n$-dimensional vector as defined by Equation (3)
$\hat{\lambda}$ = $(2m + 1)n$-dimensional vector as defined by Equation (21)
λ_m = $2mn$-dimensional vector as defined by Equation (22)
ξ = dimensionless reaction rate
τ = period of $\mathbf{y}$
φ = phase
φ^* = phase evaluated at t^*
$\mathbf{\Phi}$ = $(2m + 1)n$-dimensional vector as defined by Equation (5)
ω = frequency of $\mathbf{y}$

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Manuscript received June 4, 1969; revision received August 11, 1969; paper accepted August 15, 1969. Paper presented at AIChE New York meeting.