Small Oscillations in Undistributed Autonomous Systems

JOHN BEEK

Shell Development Company
Emeryville, California 94608

Douglas and his collaborators have in the last few years published three papers on oscillating chemical reactors. In the first (*3*), the treatment was restricted to first-order reactions, but in the second (*4*) this restriction was removed. In these papers, the useful suggestion was made that oscillations could be induced by imposing positive feedback of some quantity. In the third paper (*2*), the results of the earlier analysis were applied to observations of the behavior of an oscillating reactor. The purpose of this paper is to correct certain misunderstandings that are evidenced in these publications.

In the appendix of the second paper (*4*), Gaitonde and Douglas present a justification for dropping from the results of their analysis all terms containing third partial derivatives with respect to the dimensionless temperature, arguing that with these terms included the truncated Taylor series corresponds to a system with more than one solution of the steady state equations whereas the original system is known to provide only one solution. The authors have overlooked the fact that the truncated expansion has significance only in the neighborhood of the origin of the expansion, so that its behavior in the large is irrelevant.

The authors argue further that if these terms are retained the amplitude of the oscillation is calculated to be imaginary so there could be no oscillations, in contradiction to the observed behavior of the differential equations. In the first place, the failure to get a real value for the amplitude from such an analysis means not that there can be no oscillation, but only that there can be no small limit cycle. What happens in this case is that even when the system is only marginally unstable, the limit cycle has a large amplitude—the so-called hard oscillation. All this is set forth in the section on Poincare's bifurcation theory in "Introduction to Non-linear Mechanics" by Nicholas Minorsky (*6*).

In the second place, the behavior of the numerical solution of the differential equations must be taken into account. The curves in Figure 4 of the paper show that a small limit cycle is indeed found when the system is unstable but close to the boundary of stability. This means that the amplitude must be real, from which the conclusion is forced that there must be some error in a calculation that indicates it to be imaginary. The authors' device of omitting certain terms from their derived result to give the right qualitative behavior is not acceptable.

The method used by the authors to derive their results, multiplying the nonlinear part of the equations by a small parameter which turns out later to be unity has only heuristic value. If it leads to the right answer as verified by a valid procedure it is useful, but without verification it can not be depended upon. If one keeps in mind that the analysis is based on a truncated Taylor series, it is immediately apparent that it can be valid only for small values of the variables, which means in turn that the system, though unstable at the singular point, must be close to the boundary of stability. This means, furthermore, that the trace of the matrix of derivatives for the linearized system must be small; thus this trace gives us a quantity that determines the order of magnitude of all terms that appear in the constants of the limit cycle and so gives a basis for a consistent set of approximations. It will turn out that the limit cycle is determined with an error proportional to the three-halves power of the trace.

Andronow and Chaikin (*1*) showed how to reduce the problem of estimating the amplitude of a small limit cycle to the problem of solving a set of three recurrent linear ordinary first-order differential equations. Their procedure, applied to a Taylor series, yields an explicit expression for the amplitude in terms of the derivatives of the first three orders. This expression agrees with the one derived below. The extension of the procedure to estimate the displacement of the center of gravity from the singular point, that is, the average output, requires an unduly long and involved calculation.

A straightforward procedure that does give the displacement and also the amplitudes of the first harmonics is to express the variables in the limit cycle as harmonic series and to identify coefficients of corresponding terms in the equations resulting from substituting the series into the differential equations. This is the procedure followed by Lotka (*5*) who was however interested in the decay of a system toward a steady state instead of in a limit cycle.

The equations representing the system will be supposed to have been transformed to a standard form, as follows:

$$\dot{x} = \alpha x - \beta y + (1/2)F_{20}\,x^2 + F_{11}\,xy + (1/2)F_{02}\,y^2 + (1/6)F_{30}\,x^3 + (1/2)F_{21}\,x^2y + (1/2)F_{12}\,xy^2 + (1/6)F_{03}\,y^3 + \ldots$$

$$\dot{y} = \beta x + \alpha y + (1/2)G_{20}\,x^2 + G_{11}\,xy + (1/2)G_{02}\,y^2 + (1/6)G_{30}\,x^3 + (1/2)G_{21}\,x^2y + (1/2)G_{12}\,xy^2 + (1/6)G_{03}\,y^3 + \ldots$$

in which α is small and β is positive. A convenient transformation matrix to give this form is T in the relation

$$\begin{pmatrix} X \\ Y \end{pmatrix} = T\begin{pmatrix} x \\ y \end{pmatrix} = \begin{bmatrix} 1 & 0 \\ \dfrac{a_{22} - a_{11}}{2a_{12}} & \dfrac{-\beta}{a_{12}} \end{bmatrix}\begin{pmatrix} x \\ y \end{pmatrix}$$

where the a_{ij} are the elements of the matrix of first partial derivatives in the system

$$\dot{X} = \phi\,(X, Y)$$

$$\dot{Y} = \psi\,(X, Y)$$

and

$$\beta = 1/2\,[-4a_{12}a_{21} - (a_{22} - a_{11})^2]^{1/2}$$

This form has the advantages over the one given by Gaitonde and Douglas (*4*) that one variable is not changed, and that it reduces to the identity for a system already in the standard form.

The variables in the limit cycle are expressed as

$$x = a_1 + b_1 \cos \omega t + c_1 \sin \omega t + e_1 \cos 2\,\omega t + f_1 \sin 2\,\omega t + g_1 \cos 3\,\omega t + h_1 \sin 3\,\omega t + \ldots$$

$$y = a_2 + b_2 \cos \omega t + c_2 \sin \omega t + e_2 \cos 2\,\omega t + f_2 \sin 2\,\omega t + g_2 \cos 3\,\omega t + h_2 \sin 3\,\omega t + \ldots$$

Since the phase of ωt is arbitrary, we may assume that c_1 is small compared to b_1. On substituting these expressions into the differential equations, we find that b_1 and c_2 have the magnitude of $\alpha^{1/2}$, that the a's, e's, and f's, together with a correction on the frequency, have the magnitude of α, and that c_1, b_2, the g's and h's, and corrections to b_1 and c_2 have the magnitude of $\alpha^{3/2}$. We write

$$b_1 = b_{10} + \alpha b_{11}$$

$$c_2 = c_{20} + \alpha c_{21}$$

and

$$\omega = \beta + \alpha\omega_1$$

to make the small corrections explicit. With these modifications the balances of terms of a given sort are found to yield 18 equations grouped in four sets of 4 and one set of 2. One set of 4 gives the result $c_2 = b_1$, in addition to identities. The set of 2 and one set of 4 give expressions for the a's, e's, and f's as multiples of b_1^2. A third set of 4 gives the g's and h's as multiples of b_1^3. The last set of 4, that relating to the terms of magnitude $\alpha^{3/2}$ in the fundamental frequency, is a set of four equations linear in the unknown quantities b_1^2, ω_1, $(b_2 + c_1)/b_1$, and $(b_{11} - c_{21})/b_1$. These four equations are given in the Appendix.

In view of the fact that the coefficients of magnitude $\alpha^{3/2}$ for the fundamental frequency are not determined by this analysis, no useful purpose would be served by adding the second harmonic terms, which are of the same order of magnitude. Thus the description of the limit cycle that is obtained is restricted to the fundamental frequency, the displacement of the mean, and the first harmonic. The expressions are

$$x = a_1 + b_1 \cos \omega t + e_1 \cos 2\,\omega t + f_1 \sin 2\,\omega t + 0\,(\alpha^{3/2})$$

and

$$y = a_2 + c_2 \sin \omega t + e_2 \cos 2\,\omega t + f_2 \sin 2\,\omega t + 0\,(\alpha^{3/2})$$

with

$$b_1^2 = 16\alpha\beta/[F_{20}G_{20} - F_{02}G_{02} - F_{11}(F_{20} + F_{02}) + G_{11}(G_{20} + G_{02}) - \beta(F_{30} + F_{12} + G_{21} + G_{03})]$$

$$c_2 = b_1$$

$$a_1 = -\,(b_1^2/4\beta)(G_{20} + G_{02})$$

$$a_2 = (b_1^2/4\beta)(F_{20} + F_{02})$$

$$e_1 = (b_1^2/12\beta)(G_{20} - G_{02} - 4F_{11})$$

$$e_2 = -\,(b_1^2/12\beta)(F_{20} - F_{02} + 4G_{11})$$

$$f_1 = (b_1^2/6\beta)(F_{20} - F_{02} + G_{11})$$

$$f_2 = (b_1^2/6\beta)(G_{20} - G_{02} - F_{11})$$

$$\omega = \beta + (b_1^2/48\beta)[-2F^2_{20} - 2G^2_{02} - 5F_{02}(F_{20} + F_{02}) - 5G_{20}(G_{20} + G_{02}) + F_{11}(G_{20} + 5G_{02} - 2F_{11}) + G_{11}(5F_{20} + F_{02} - 2G_{11}) - 3\beta\,(F_{21} + F_{03} - G_{30} - G_{12})]$$

A striking difference between these expressions and those given by Gaitonde and Douglas (*4*) is that no terms involving second-order derivatives appear in their expressions for the amplitude of the fundamental or for the correction to the frequency.

The hypothetical system studied by Warden, Aris, and Amundson (*7*) provides a good example for the application of the results of this paper. In dimensionless form, their equations may be expressed as follows:

$$\dot{X} = (1/2)(E - 1) - X(E + 1) + (1/2)X^2 E$$

and

$$\dot{Y} = (1/2)XE - (1/4)X^2E - Y\left(2 + \frac{k}{8}\right) + kY^2 - (1/4)(E - 1)$$

in which

$$E = \exp\,[25Y/(Y - 1)]$$

The trace of the matrix for the linearized system is $(18 - k)/8$, so the boundary of stability is at $k = 18$. The numerical results given are for $k = 17.99$. We find for the limit cycle

$$10^4X = 3.94 + 336.99 \cos \omega t - 449.32 \sin \omega t - 19.93 \cos 2\,\omega t - 38.28 \sin 2\,\omega t$$

and

$$10^4Y = 2.21 + 112.33 \sin \omega t + 9.99 \cos 2\,\omega t + 4.52 \sin 2\,\omega t$$

where

$$\omega = 1.49737$$

The trajectory given by these expressions was compared with the solution of the differential equations, using the constants of the calculated cycle to give the positive value of X for a zero value of Y and to give the time for the return to the initial point. The following table shows the correspondence between the two sets of results, with eight points equally spaced in time around the cycle.

From Harmonic Series		From Differential Equations, Using ω	
10^2X	10^2Y	10^2X	10^2Y
3.7436	−0.0066	3.7132	0.0000
−0.5869	0.7942	−0.5272	0.7755
−3.9626	1.0509	−3.9277	1.0511
−5.1574	0.8299	−5.1750	0.8315
−3.8959	0.2275	−3.8624	0.2182
−0.1657	−0.6202	−0.2160	−0.6016
4.2737	−1.1835	4.2219	−1.1809
6.0078	−0.9156	6.0841	−0.9167
(3.7436)	(−0.0066)	3.7126	0.0000

The best way to test the effectiveness of the harmonic representation used is to examine the root mean square contribution of each step in the approximation. X is taken for an example. The root mean square contributions of the fundamental and of the first harmonic can be calculated directly from the coefficients. Values of the contributions of all even harmonics and of all odd harmonics beyond the first can be calculated from the discrepancies between the approximate and correct values of X. If we denote these discrepancies as $Z(\omega t)$, the magnitude of the sum of the even harmonics is given by

$$1/2 \mid Z(\omega t) - Z(\omega t + \pi) \mid$$

and the magnitude of the sum of the odd harmonics beyond the first by

$$1/2 \mid Z(\omega t) + Z(\omega t + \pi) \mid$$

The root mean square values of these quantities clearly give upper-bound estimates of the root mean square contributions of the second and third harmonics, respectively. The estimates were formed from values of Z calculated at 48 equally spaced points in the cycle. The resulting estimates of the contributions of the fundamental and the first three harmonics are found to be

$$397.15 \times 10^{-4},\ 30.77 \times 10^{-4},\ 3.95 \times 10^{-4},\ \text{and } 0.51 \times 10^{-4}.$$

These values progress by factors of about 0.1, which is to be compared with the value of $\alpha^{1/2}$, 2.5×10^{-2}. Presumably, the functions of the derivatives account for the difference.

The accuracy achieved in the approximations in this example should not be taken to mean that the expressions given above can be expected to give accurate estimates of the constants of a cycle that is not really small. If in the system treated above, we take $k = 16$, which gives a limit cycle with X oscillating between -0.26 and 0.74, the harmonic approximation gives a double loop with X extending from -0.95 to 1.73.

A QUALITATIVE CRITERION FOR OSCILLATORY SYSTEMS

The quantity that appears in the denominator of the expression for b_1^2 is an important criterion for characterizing the behavior of systems which are near a boundary of oscillatory instability. We have seen above that when this quantity is positive, a system that is marginally unstable undergoes a small oscillation, whereas when it is negative, the system goes into a large oscillation, which may be bounded only by the constraints on the system. The importance of the criterion is magnified by its significance in systems that are on the stable side of the boundary. Here the trace is negative, so that the amplitude of the limit cycle is real when the criterion is negative, but, since the singular point is stable, the cycle is unstable; it is, in fact, the boundary of the region of asymptotic stability. This means that for such a system, the region of asymptotic stability shrinks to nothing as the system approaches the boundary of stability, a situation that is to be avoided. When the criterion is positive, on the other hand, the region of asymptotic stability does not become small when the system approaches the boundary of stability. Thus, on either side of the boundary of stability a system behaves well if the criterion is positive and ill if it is negative.

This criterion should not be thought of as an approximation that would be changed if higher derivatives were taken into account. No higher derivatives can affect the qualitative behavior close to the boundary of stability if the criterion is not zero. Strictly speaking, nevertheless, it is true that the criterion should be evaluated for a neutrally stable system. The only possibility for confusion comes from a change of sign of the criterion between the boundary of stability and the case being studied which, in view of the requirement that the system be close to the boundary, would mean that the criterion would be close to zero.

NOTATION

a_{ij} = elements of the matrix for the linearized system
a_1, a_2 = mean values of x and y in a cycle
b_1, b_2 = coefficients of cos ωt in the approximation
$b_{10}, b_{11} \times b_1 = b_{10} + \alpha b_{11}$
c_1, c_2 = coefficients of sin ωt
$c_{20}, c_{21} \times c_2 = c_{20} + \alpha c_{21}$
e_1, e_2 = coefficients of cos 2 ωt
E = exp $[25Y/(Y - 1)]$
f_1, f_2 = coefficients of sin $2\omega t$
F_{ij} = $\partial^{i+j}(\dot{x})/\partial x^i \partial y^j$
G_{ij} = $\partial^{i+j}(\dot{y})/\partial x^i \partial y^j$
k = a parameter in the numerical example
T = transformation matrix
x, y = transformed state variables
X, Y = state variables
Z = error in an estimate of a variable
α = one-half the trace of the matrix for the linearized system, a small quantity
β = angular frequency in the linearized system
ω = estimated angular frequency of the oscillation
ω_1 = $\omega = \beta + \alpha\omega_1$

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APPENDIX

The four equations representing balances of the coefficients of cos ωt and sin ωt having the magnitude of $\alpha^{3/2}$ are shown below with b_1 substituted for c_2 where it appears.

$$-\beta \frac{b_2 + c_1}{b_1} + 1/2\ b_1^2 \left[F_{20} \frac{2a_1 + e_1}{b_1^2} + F_{11} \frac{2a_2 + e_2 + f_1}{b_1^2} + F_{02} \frac{f_2}{b_1^2} + 1/4\,(F_{30} + F_{12}) \right] = -\alpha$$

$$\beta \frac{b_2 + c_1}{b_1} + 1/2\ b_1^2 \left[G_{20} \frac{f_1}{b_1^2} + G_{11} \frac{2a_1 - e_1 + f_2}{b_1^2} + G_{02} \frac{2a_2 - e_2}{b_1^2} + 1/4\,(G_{21} + G_{03}) \right] = -\alpha$$

$$\omega_1 + \beta \frac{c_{21} - b_{11}}{b_1} = 1/2 \frac{b_1^2}{\alpha} \left[G_{20} \frac{2a_1 + e_1}{b_1^2} + G_{11} \frac{2a_2 + e_2 + f_1}{b_1^2} + G_{02} \frac{f_2}{b_1^2} + 1/4\,(G_{30} + G_{12}) \right]$$

$$-\omega_1 + \beta \frac{c_{21} - b_{11}}{b_1} = 1/2 \frac{b_1^2}{\alpha} \left[F_{20} \frac{f_1}{b_1^2} + F_{11} \frac{2a_1 - e_1 + f_2}{b_1^2} + F_{02} \frac{2a_2 - e_2}{b_1^2} + 1/4\,(F_{21} + F_{03}) \right]$$