Multiple Limit Cycles in a CSTR

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In a recent paper Heberling et al. (1971) noted the most interesting feature of the existence of an unstable limit cycle surrounded by a stable limit cycle in a model representing the behavior of a CSTR. The purpose of this communication is to comment further on the analysis of this system and to show that essentially all of the currently available methods are inadequate to define the system.

The model used by Heberling et al. to describe the reactor of Gaitonde and Douglas (1969) is

$$\frac{dx_1}{dt} = -x_1 - \beta_1 [1 - (1 - x_1)k] \quad (1)$$

$$\frac{dx_2}{dt} = -\beta_4 x_2 + \beta_5 [1 - (1 - x_1)k] \quad (2)$$

with

$$k = \exp\left[\frac{\beta_3 x_2}{x_2 - 1}\right] \quad (3)$$

where x_1 represents the negative deviation from dimensionless steady state concentration and x_2 represents the negative deviation from dimensionless steady state temperature. We wish to analyze the reactor performance which corresponds to the choice of the parameters to give Figure 4 of Heberling et al. (1971). Taking $\beta_3 = 80.0$ and the other conditions of operation from Case 3 of Gaitonde and Douglas, we obtained the parameters $\beta_1 = 2.5088$, $\beta_4 = 21.552$, and $\beta_5 = 0.31281$. These values differ only slightly from those of Heberling et al.; this is most likely due to our use of double precision in doing the calculations.

With this choice of the parameters, the system described by Equations (1) and (2) exhibits two limit cycles as is shown in Figure 1. Both the stable and the unstable limit cycles are very slightly larger than the corresponding limit cycles given by Heberling et al. The agreement, however, is sufficiently good to enable us to use the above values for the parameters for the analysis and to provide a direct comparison.

The first step in the analysis is to approximate the nonlinear exponential function given in Equation (3). Since x_2 is very small in comparison to 1.0, we may approximate k in Equation (3) by

$$k = \exp(-\beta_3 x_2) \quad (4)$$

with essentially no loss of accuracy in the result.

QUADRATIC APPROXIMATION FOR k

Let us now approximate k given by Equation (4) by the truncated Taylor series expansion

$$k = 1 - \beta_3 x_2 + \frac{\beta_3^2 x_2^2}{2} \quad (5)$$

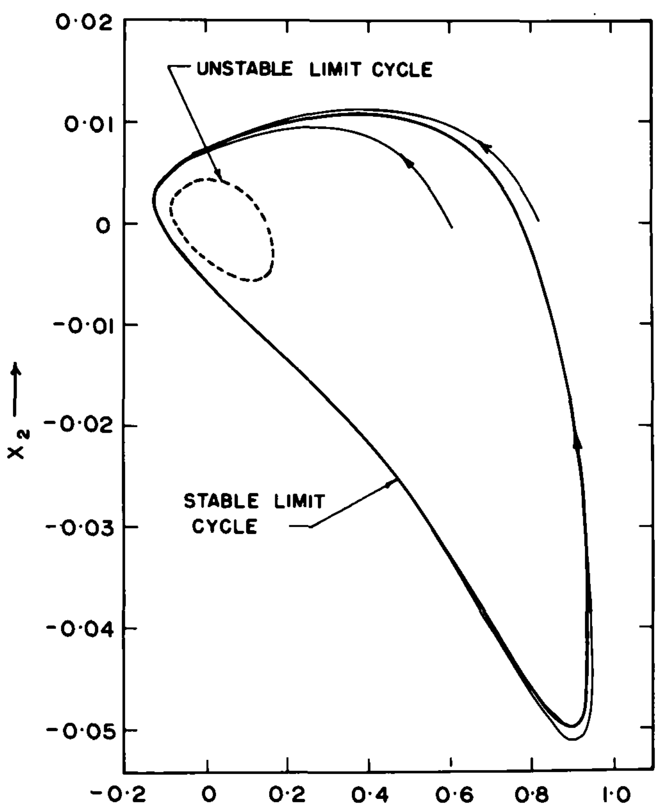

Fig. 1. Phase plane with actual value of k

$$k = \exp\left[\frac{\beta_3 x_2}{x_2 - 1}\right]$$

Substitution of Equation (5) into Equations (1) and (2) and the application of the averaging technique of Luus and Lapidus (1966) yields immediately

$$\frac{dr}{dt} = \frac{r}{2}\left[-(1 + \beta_1 - \beta_3\beta_5 + \beta_4) - \frac{\beta_1\beta_3^2r^2}{4} \right] \quad (6)$$

Substituting the numerical values for the parameters gives

$$\frac{dr}{dt} = \frac{r}{2}[-0.0359 - 4000\,r^2] \quad (7)$$

Equation (7) predicts that the system is asymptotically stable and no limit cycles exist. This was confirmed by numerically integrating Equations (1) and (2) with k given by Equation (5) to give the phase plane in Figure 2.

CUBIC APPROXIMATION FOR k

When we include an additional term in the Taylor series expansion, namely,

$$k = 1 - \beta_3x_2 + \frac{\beta_3^2x_2^2}{2} - \frac{\beta_3^3x_2^3}{6} \quad (8)$$

and apply the averaging technique, we get

$$\frac{dr}{dt} = \frac{r}{2}\left[-(1 + \beta_1 - \beta_3\beta_5 + \beta_4) - \frac{\beta_1\beta_3^2r^2}{4} + \frac{\beta_5\beta_3^3r^2}{8} \right] \quad (9)$$

Substituting in the numerical values for the parameters gives

$$\frac{dr}{dt} = \frac{r}{2}[-0.0359 - 4000\,r^2 + 20{,}000\,r^2] \quad (10)$$

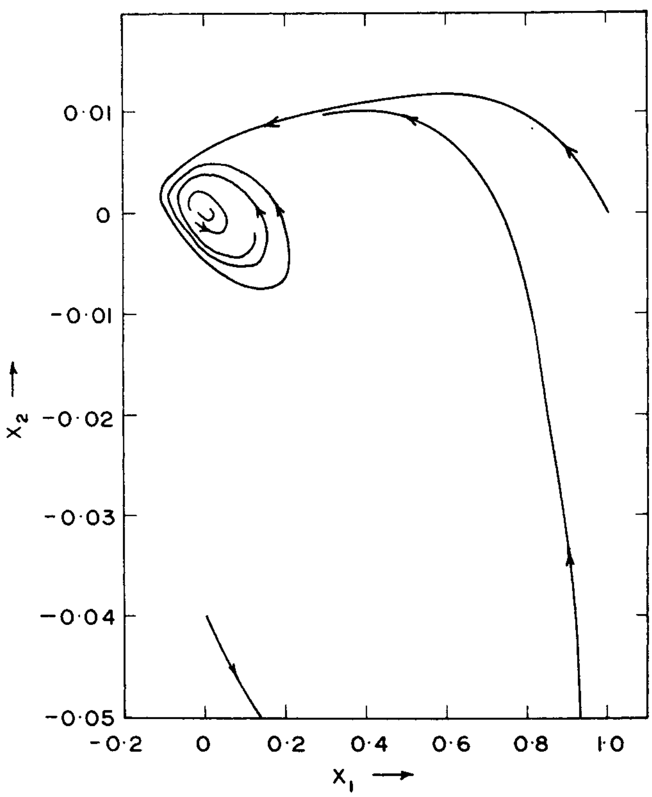

Fig. 2. Phase plane with quadratic approximation for k

$$k = 1 - \beta_3x_2 + \frac{\beta_3^2x_2^2}{2}$$

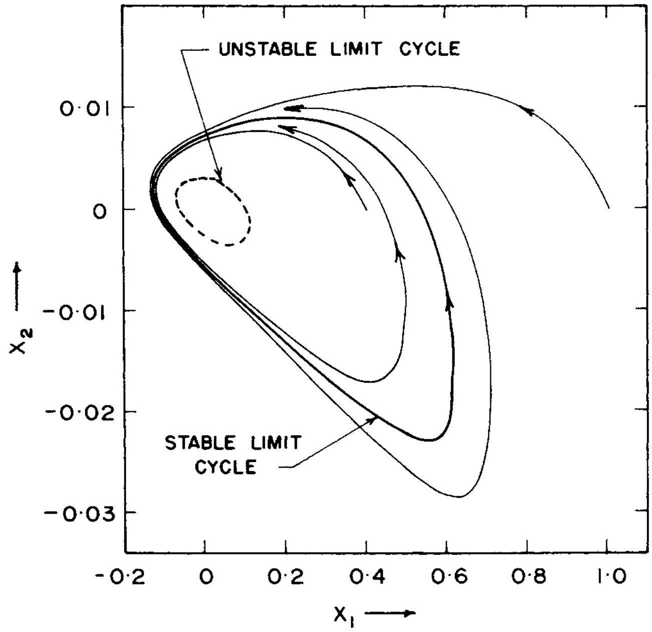

Fig. 3. Phase plane with cubic approximation for k

$$k = 1 - \beta_3x_2 + \frac{\beta_3^2x_2^2}{2} - \frac{\beta_3^3x_2^3}{6}$$

which predicts an unstable limit cycle of radius

$$r = 1.5 \times 10^{-3} \quad (11)$$

Numerical integration of Equations (1) and (2) with k given by Equation (8) yielded not only an unstable limit cycle (expected), but also a stable limit cycle surrounding the unstable limit cycle. The phase plane is shown in Figure 3. The radius of the unstable limit cycle is approximately 1.6×10^{-2} which is somewhat greater than predicted by Equation (11). In applying the averaging technique we have not used any scaling or transformation of the variables, so that x_1 and x_2 are treated alike.

When a fourth-order expansion is used for k, the use of the averaging technique leads us to expect an unstable limit cycle inside a stable limit cycle. The expected radii are, however, in great error. As higher order terms are used, the scaling becomes increasingly important. We shall consider the effect of scaling and transformation in the use of the averaging technique in a later paper.

Heberling et al. (1971), in their analysis based on the elimination of secular terms, had to use a fifth-order expansion for the nonlinear functions (that is, a fourth-order expansion for k) in order to establish the existence of two limit cycles. Since the two limit cycles are already present with the third-order expansion of k, it is apparent that this method, as well as the averaging technique, is really not adequate as currently used. We shall however comment further on this in a later paper.

LITERATURE CITED

Gaitonde, N. Y., and J. M. Douglas, "The Use of Positive Feedback Control Systems to Improve Reactor Performance," *AIChE J.*, 15, 902 (1969).

Heberling, P. V., N. Y. Gaitonde, and J. M. Douglas, "Multiple Limit Cycles in a CSTR," *ibid.*, 17, 1506 (1971).

Luus, R., and L. Lapidus, "An Averaging Technique for Stability Analysis," *Chem. Eng. Sci.*, 21, 159 (1966).

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